

## PhD Position: Liquid state NMR experiments using a dedicated DNP NMR spectrometer based on a unique dual centre magnet

The Dynamic Nuclear Polarisation (DNP) research group in Nottingham has designed and built a unique prototype DNP NMR facility based on a magnet with two iso-centres (3.4T and 9.4T)<sup>1</sup>. Hyperpolarised spin systems can be prepared by low temperature DNP (1.4K) at the 3.4T isocentre.<sup>2</sup> Subsequently the sample is shuttled in solid state to the high field centre and rapidly dissolved by injection of small amounts of hot water. After this temperature jump the sample containing the highly polarised molecules is in liquid state at ambient temperature. The resulting signal enhancement compared to a thermally polarised sample which is used in conventional NMR can reach more than  $10^4$ .

This strategy makes it possible to detect either molecules at very low concentration or acquire their NMR signal in a single excitation even for  $^{13}\text{C}$  NMR.

The project involves the investigation and improvement of several aspects of the experimental protocol:

a) Testing novel radicals for their DNP properties. In particular, we are interested to develop strategies to increase the polarisation built-up time so that the overall waiting time for the generation of highly polarised samples can be substantially reduced.

b) Testing novel ideas to decrease the volume of hot water needed to dissolve the cold sample. In particular, we will investigate the use of infrared lasers and microwaves to assist the melting and dissolution of the sample.

c) Designing new ideas to mix samples in liquid state rapidly. The motivation is to use highly polarised ligands and monitor binding of these small molecules to larger macromolecules.

d) Application of the improved strategy to study model ligand- protein systems to measure binding constants, first site of approach etc.

This project requires an interest in experimental physics and offers training in a very wide range of techniques, including spin dynamics investigations, the testing of novel NMR hardware components and the application of novel NMR strategies to studies of biomolecular model systems.

The DNP group in Nottingham currently carries out research in DNP NMR theory and hardware development. It has recently received a prestigious Novel Technology Development award by the EPSRC that fund research with the objective to optimise the dissolution DNP NMR strategy.

### References:

1. Leggett, J et al. Phys. Chem. Chem. Phys. 12(22), 5883-5892, 2010
2. Ardenkjaer-Larson et al. 2003, Proc. Natl. Acad. Science USA, 100(18) 10158

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The Centre for Doctoral Training in Integrated Magnetic Resonance (iMR) is a collaboration between researchers at the Universities of Warwick, St Andrews, Southampton, Aberdeen and Nottingham.