

Dynamic Nuclear Polarisation a New Frontier in Magnetic Resonance of Solids

Summary

This project seeks to develop a new generation of Dynamic Nuclear Polarisation (DNP) magnetic resonance (MR) spectrometer with unparalleled versatility and frequency range of operation which will open up new areas of application for MR through huge gains (10^2 - 10^3) in signal sensitivity. The project team of academic and industrial scientists has a world-leading blend of expertise, with a core team of Ray Dupree, Andy Howes, Julie Macpherson (Chemistry), Mark Newton, Kevin Pike (Project Manager), Mark Smith, and Pat Unwin (Chemistry) at Warwick and numerous collaborators in over a dozen locations worldwide.

The Warwick team has well established track records in both nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR). There are two distinct strands of expertise in the collaborators: (i) development of novel, leading-edge MR hardware, and (ii) application in areas of scientific research where the new experimental technology will provide key, novel insight into the problems. We are looking for a whole range of PhD students to start work on the D²NP project. The projects include:

Novel Probe Development

Mark Smith, Mark Newton, Ray Dupree, Andy Howes and Kevin Pike

The heart of any solid state NMR experiment is the probehead that contains the sample. To accomplish this DNP experiment several potential methodologies could be employed. There is simply irradiating the sample with high power microwaves to force the electron transitions and thereby encourage the nuclear transitions to bring about the enhanced signal. This in itself is a challenge as it requires a probe that will spin at low temperature (i.e. < 100K) and allow access of the microwaves to the sample. An alternative approach is to try and make the probes doubly resonant. This will be a significant technological challenge, but offers a number of exciting advantages. There is the potential for this project to be carried out in collaboration with an internationally leading probe manufacturing company



Applications of DNP to Biomolecular Chemistry

Mark Smith, Ray Dupree, Andy Howes and Kevin Pike

During the last decade many new developments in solid state NMR have resulted in the resolution of membrane protein structural details. A major problem is sensitivity because of the limited amount of material and its 'dilution'. DNP enhancement would allow solid state NMR on much larger proteins; it would make 2D experiments more feasible, thus giving new structural information, and would also allow 'unusual' nuclei such as ¹⁷O, ²⁵Mg, ⁶⁷Zn, etc. to be studied opening up a whole range of previously inaccessible biomolecules for investigation. This project will involve the development and implementation of pulsed DNP experiments at high magnetic fields, their optimisation and application to the investigation of protein structures using NMR and DNP.

Defect-controlled Properties of Materials

Mark Newton, Kevin Pike, Andy Howes, Ray Dupree and Mark Smith

In materials containing both magnetic nuclei and unpaired electrons (to act as the polarisation source), DNP combined with modern solid-state NMR spectroscopy can be used to study properties that could not be investigated by NMR spectroscopy alone. The polarisation source may be produced by a variety of techniques ensuring that DNP/NMR will be a versatile technique for the study of a variety of materials. This project will involve the implementation of pulsed DNP experiments at as high field as possible with new sequences, and the investigation of defect-controlled properties with pulsed EPR, NMR and DNP in a variety of insulator and semiconductor materials.

Electrochemical Magnetic Resonance Studies

Mark Newton, Julie Macpherson (Warwick Chemistry) and Pat Unwin (Warwick Chemistry)

Magnetic resonance has long been recognized as a powerful technique for in-situ spectroscopic characterisation of electrode reactions, but not widely exploited due to experimental constraints. With the exceptional detection sensitivity of the new EPR instrumentation, and unprecedented sensitivity gains in NMR using DNP, we have a unique opportunity to radically re-think the approach to in-situ electrochemical EPR and DNP/NMR spectroscopy. The project will involve the development of new magnetic resonance - electrochemical probes which will be used to study, for example, semiconductor-liquid interfaces.

Catalysis and Fuel Cell Applications

Mark Smith, Kevin Pike and Dave Thompsett (Johnson Matthey Research).

Understanding surface structures and features that affect catalytic processes (such as in exhaust emissions), and the influence of electrolyte and electrode structure on the performance of fuel cells are parts of key technologies underpinning new power sources and greener technology. NMR could play a direct role in these areas through the increased sensitivity afforded by DNP. The project will involve application of NMR to the study of catalytic processes, development of techniques for DNP enhancement of surface species and construction of a cell for in situ DNP operation based around a micro-reactor. This project will develop *in situ* catalytic reactors for the spectrometer using the expertise of Johnson Matthey Research who will be a partner in this project

If interested in any of these projects please contact Mark Smith (m.e.smith.1@warwick.ac.uk), Mark Newton (m.e.newton@warwick.ac.uk), Ray Dupree (ray.dupree@warwick.ac.uk) or Kevin Pike (Kevin.Pike@warwick.ac.uk).