

PhD Position: High pressure electron magnetic resonance

Despite its fundamental importance pressure is a rather neglected variable in magnetic resonance experiments. Applying uniaxial stress to materials paramagnetic centres can provide unique information, it can break symmetry allowing centre symmetry ambiguities to be resolved, and for high symmetry centres it can allow the spin state to be determined, for example the isotropic Ga vacancy spectrum in GaP was shown to be $S = 3/2$. In addition, current semi-empirical models for calculating spin-Hamiltonian zero-field splitting terms require parameters obtained from pressure dependent EPR measurements on 'model' high symmetry transition-ion doped host crystals. The application of stress is of particular value in the study of defect centres in diamond and other semiconductors, and in piezoelectric materials.

This project is a collaboration with Prof. Mark Newton, University of Warwick, and aims to develop and implement diamond anvil pressure cells in loop-gap EMR resonator structures for high pressure EPR studies of materials. Development of high pressure cells has been pioneered at Warwick where they have been used to perform Raman measurements on diamond, applying uniaxial stresses up to approximately 4 GPa. However, further work is required before the technology can be translated to allow routine EPR measurements. An expected outcome of the project is that high pressure EPR resonators will be implemented and tested, one for operation with spectrometers at Dundee and St Andrews and one at Warwick, initially at 9.5 GHz but a further aim will be to investigate extending the technology to 34 GHz. An additional technological challenge to be approached will be to combine a high pressure cell with a cryostat for low temperature EPR measurements. A further possible aim will be to investigate the design and implantation of a hydrostatic pressure cell.

In addition, the first high pressure EPR experiments have been reported that have investigated conformational equilibria in proteins so, for example, gaining insight on protein folding. A similar high pressure system is being assembled at Dundee. In consequence, the student involved in technological development of high pressure cells for materials EPR application can also provide input to technique development for pressure dependent biophysical EPR.

The PhD student will be based at the University of Dundee under the supervision of Dr David Keeble (d.j.keeble@dundee.ac.uk) (01382 384561).

For further information contact David Keeble or iMR.CDT@warwick.ac.uk

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