Research cluster potential projects: Catalysis

Supervisors

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Projects

Project Title: NMR Analysis of Soft Solid Low Molecular Weight Gelator (LMWG) Hydrogels
Supervisor(s): Dr J A Iggo and Dr D J Adams (Materials)
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Measurement of the macroscopic properties of gels is relatively easy but determining the molecular interactions leading to gel formation; the dimensions of the pore structure formed by the entangled LMWG fibres; and the diffusivity of guests within the gel is difficult at the microscopic level. This project will develop non-invasive NMR methods to probe the aggregation and self-assembly processes, and the environments and interactions between different sites on the LMWGs (e.g. H-bonding via Δδ and nOe), as well as the analysis of changes in diffusion of the species present during gelation and within the formed gel (via DOSY measurements).

Project Title: High pressure NMR investigation of the response of muscle kinases to applied force
Supervisor(s): Dr J A Iggo Dr O Mayans (Structural and Chemical Biology)
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Mechanical stimulation through exercise is critical to the development and regeneration of muscle tissue. Giant, elastic proteins in the muscle fibres act as key transducers of mechanical signals in this process. This project will employ High Pressure $^{31}$P NMR to profile the activity of these kinases in vitro under strain-mimicking conditions, monitoring the fate of phospho-groups in the kinase substrates and products as a function of pressure and will study the dynamics of mechanosensitive regulatory regions by heteronuclear NMR.
Oxidation is one of the most fundamental and widely-used reactions in chemical, pharmaceutical and materials synthesis. An oxidant, such as metal peroxides, hydrogen peroxide or oxygen gas, is almost always used, which incurs considerable safety issues and in many cases generates copious waste. An alternative method is to remove hydrogen via dehydrogenation. However, few catalysts are known that allow easy dehydrogenation. We have recently discovered a range of metal complexes that show considerable activity in dehydrogenation reactions. This project aims to develop the catalysts and underlying mechanism, targeting reactions of fundamental and commercial significance.

Amines are key molecules for pharmaceutical, agrochemical, fine chemical and materials synthesis. Reductive amination is a best way for accessing amines and a key green chemistry research area according to the American Chemical Society Pharmaceutical Roundtable. We have recently discovered catalysts that allow for efficient reductive amination, some of which have already found commercial applications. This project aims to develop the chiral version of these catalysts such that they can be used for asymmetric direct reductive amination to give chiral secondary as well as primary amines. The project involves close collaboration with the pharmaceutical industry. commercial significance.

This project will explore innovative methods to enable asymmetric catalysis, an area of vital importance to chemical, pharmaceutical and materials synthesis, which has been dominated with expensive, toxic metals and ligands. Focusing on asymmetric reduction or C-C bond formation, you will develop molecular catalysts based on cheap, safe metals and on ligands that are modular and easy to access. The project will make use of homogeneous catalysis, organometallic chemistry, organic chemistry, and mechanistic studies, and involve collaboration with the pharmaceutical industry.
**Project Title: Characterization of Supramolecular Complexes in Cooperative Catalysis**

Supervisor(s): Dr J A Iggo, Prof J L Xiao and Dr N Berry (Organic)

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The unification of organometallic with organic catalysis creates an exciting new reaction space – cooperative catalysis – in which the substrates of a reaction are activated simultaneously by electronic and steric interactions with the metal and by non-covalent interactions, such as hydrogen bonding, electrostatic, π–π, CH-π and hydrophobic forces, enabling reactivity and selectivity patterns inaccessible within each of catalysis field alone. This project will use NMR methods (nOe, PFGSE diffusion measurements, etc) to explore the mechanisms by which the two catalysts interact cooperatively through a supramolecular assembly of catalysts and substrate, bound together by non-covalent interactions.

**Project Title: Selective, efficient and clean chemical hydrogenation using new electrochemical catalysts**

Supervisor(s): Professor Richard J. Nichols (Applied Physical) and Professor Jianliang Xiao

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This PhD studentship is in a new research area which involves the development and understanding of molecular electrochemical catalysts for synthesis. The project will involve both the synthesis of molecular catalysts for attaching to surfaces as well as measurements and electrochemical synthesis. A primary aim is to demonstrate that electrochemistry can be used with surface grafted molecular catalysts to selectively, efficiently and cleanly achieve hydrogenation reactions which are usually carried out using solution phase homogeneous catalysis or with heterogeneous catalysts under high pressure. The studentship will promote a range of interdisciplinary skills including synthesis, catalysis, electrochemistry and measurement techniques.