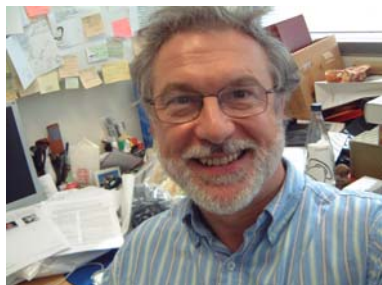




**Professor Colin Bain**  
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Colin Bain graduated in Natural Sciences from Cambridge before crossing the Atlantic to undertake his PhD at Harvard with Prof. George Whitesides. He then returned to Cambridge as a Royal Society Fellow, working with Dr. Paul Davies to set up the UK's first sum-frequency spectrometer. In 1991 he moved to Oxford as a University Lecturer and Fellow of Magdalen College. In 2005 he took up his current position of Professor of Chemistry at Durham University. His research interests lie principally in the chemistry and physics of interfaces, with applications in detergents, personal care products, printing, spraying and lubrication. Prof. Bain has received the Harrison, Corday-Morgan and Tilden Prizes from the Royal Society of Chemistry as well as awards in Japan and Australia. In 2005 he was honoured to deliver the annual McBain Lecture at the National Chemical Laboratory in Pune. He has collaborated with the Indian Institute of Science in Bangalore for a number of years and currently holds a joint UKIERI award with the IISc. Since 2008, he has been a Director of the Institute of Advanced Study at Durham – an institute that seeks to promote interdisciplinary dialogue and research collaborations across the humanities, sciences and social sciences. He has been actively involved in many aspects of industry-academia interactions, through research collaborations with industry, as a Director of the Oxford Science Park and as a scientific advisor to a venture capital partnership.



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HAGAN BAYLEY is the Professor of Chemical Biology at the University of Oxford. He enjoys working at the interface of chemistry and biology by, for example, developing techniques for protein modification that have applications in both basic science and biotechnology. He received his B.A. in chemistry from Oxford in 1974, while at Balliol College, and his Ph.D. in chemistry from Harvard University in 1979 in the laboratory of Jeremy Knowles. After postdoctoral work with Gobind Khorana at the Massachusetts Institute of Technology, he was on the faculty at Columbia University and the University of Oxford. From 1988 to 1996, he was at the Worcester Foundation for Experimental Biology in Shrewsbury, Massachusetts, and from 1997 to 2003 at Texas A&M University in College Station. Dr. Bayley has published about 200 papers in journals including Science and Nature. His laboratory's work on the engineering of membrane pores has received widespread attention and in 1997 it was described in an article in Scientific American. Recently, the development of engineered pores for stochastic sensing, the rapid screening of membrane proteins, the study of covalent chemistry at the single molecule level and ultrarapid DNA sequencing have become major interests of the laboratory. In 2005, Dr. Bayley founded Oxford Nanopore Technologies to exploit the potential of stochastic sensing technology.



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Alejandra Palermo graduated as a chemical engineer (Argentina) and her undergraduate studies included a period at the Chemical Engineering Department of the University of Sao Paulo, Brazil. Her subsequent PhD research in Materials Science dealt with theoretical and experimental studies of diffusion of high molecular weight hydrocarbons in zeolites. She went on to become an Assistant Professor in Chemical Engineering (UNMDP, Argentina) before joining the Chemistry Department at Cambridge University under a Royal Society Visiting Fellowship. She was subsequently awarded the position of CONICET External Research Fellow and for the next 7 years she continued to work in Cambridge in the field of heterogeneous catalysis and surface science. She has over 50 publications in the area of diffusion, heterogeneous catalysis, solid state electrochemistry and surface science, including synchrotron radiation methods. In 2002 she joined the RSC as Project Manager for the *International Review of UK Chemistry* and after this worked on the follow-up action plan based on the recommendations of the IRC report, particularly in science policy activities on sustainable chemistry, national security and the development of the chemistry/chemical engineering interface. Since 2006, her work is focused on the development of international research collaborations. In 2007 she was appointed RSC Manager for the Pan African Chemistry Network. She is a member of the IUPAC task in *International Research Funding in the Chemical Sciences* project, a Fellow of the RSC and of IUPAC, and a member of the IChemE. She is member of the steering group that authored the PACN report on "Africa's Water Quality", launched on World Water Day in March 2010.



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Hugo Vits is currently the Bitumen Technology Manager, Site and HSSE Manager Bangalore Technology Centre, for Projects & Technology in Shell.

He has 18 years experience in a variety of roles in the energy industry - including R&D site management, innovation management, commercial and regulatory management, business acquisition and restructuring in Europe, Latin America and Asia).

Hugo holds a PhD in Chemical Engineering (U of Minnesota, USA) and a Chemical Engineering Diploma (U of Concepcion, Chile). He has published technical papers in biotechnology and environmental science.



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Thomas Faust graduated with a master's degree from the University of Sheffield (UK), where his research concerned the solvothermal synthesis of octametallic coordination cages, with a view to investigating host-guest and related properties. Upon finishing in 2008, he moved across The Pennines to The University of Manchester (UK) where he was awarded a MAGMANet (EU) / EPSRC (UK) Early Researcher Fellowship, and continues to pursue a European Doctorate. His work here involves design, synthesis, characterisation and measurement of cyclic heterometallic clusters and arrays of clusters towards potential applications including the clean-up of radioactive contaminated waters and quantum information processing systems. His specialities include  $^1\text{H}$  NMR of large paramagnetic clusters and single crystal x-ray diffraction including the use of synchrotron light. Thomas also spent a period in 2009 at the Institute for Molecular Science, University of Valencia (SPAIN), where he was investigating molecular switches for incorporation into linked-cluster systems.

# ACHIEVING SPIN ENTANGLEMENT BETWEEN MOLECULAR NANOMAGNETS - a lead into quantum information processing

Thomas B. Faust and Richard E. P. Winpenny

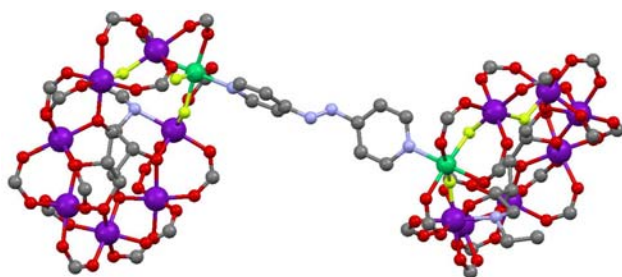
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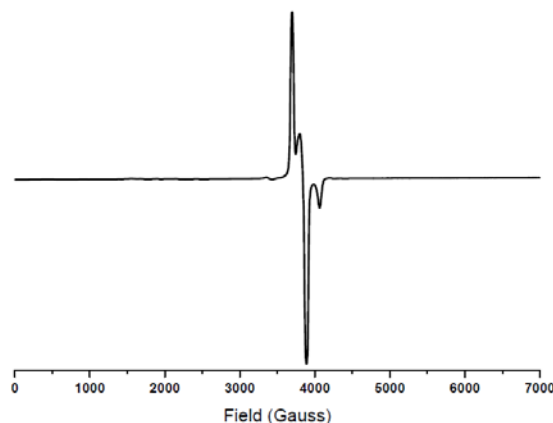
A recent focus of my work has been the synthesis of octametallic cyclic arrays of antiferromagnetically superexchanging, paramagnetic metal centres. It has been proposed that these molecular “wheels” could be used as qubits in quantum information processing.<sup>[1]</sup> Chemical versatility of these clusters has allowed their functionalisation, thereby giving a handle by which two or more such clusters can be linked via covalent bonding.

The nature of the interwheel link determines whether entanglement of the individual spin states of the wheels is observed. The magnetic communication is determined, and to some extent quantified, using low temperature electron paramagnetic resonance spectroscopy (EPR).<sup>[2]</sup>

EPR shows the weak magnetic exchange between two  $S = \frac{1}{2}$  subsystems in  $\{\text{Cr}_7\text{Ni}\}\text{azpy}\{\text{Cr}_7\text{Ni}\}$  (see **Fig 1.**) in the creation of a spin triplet (see **Fig. 2.**).



**Figure 1: Two  $\{\text{Cr}_7\text{Ni}\}$  wheels ( $S = 1/2$ )  
linked via 4,4'-azopyridine (azpy)**



**Figure 2: EPR X-Band (9.25 GHz) powder spectrum at  
5 K of the compound in Figure 1**

[1] Richard E. P. Winpenny et al., “Molecular engineering of antiferromagnetic rings for quantum computation.” *Phys. Rev. Lett.*, 2005, **94**, 207208

[2] Marco Affronte et al., “Entanglement in supramolecular spin systems of two weakly coupled antiferromagnetic rings (purple- $\text{Cr}_7\text{Ni}$ )”, *Phys. Rev. Lett.*, 2010, **104**, 037203



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Nick Brooks graduated in 2002 from the University of Cambridge with a degree in Natural Sciences, specialising in Chemistry. He then moved to Imperial College London for a PhD in soft matter chemistry, researching mesoporous catalyst formation using self assembled metallo-surfactant templates. After completing his PhD, Nick began work as a research associate at Imperial, working on projects including 'Recognition of double stranded DNA' and 'Micromechanics of living cells'. He is now senior post-doc in the Membrane Biophysics Platform Group and has recently been leading research in a collaborative project to develop a national user facility for pressure jump X-ray diffraction experiments, working with colleagues at Imperial and Diamond Light Source—the new UK synchrotron.

In addition to research work, Nick has been heavily involved in early career researcher development, improving resources for professional development within the Department of Chemistry and Imperial College as a whole. He represents the Department of Chemistry and Faculty of Natural Sciences on the Imperial College post doctoral development advisory committee, has contributed to the Department of Chemistry application for an Athena Swan silver award and has established a departmental early career development group aimed at offering improved development opportunities and promoting internal and external networking. He also has a strong interest in science communication and has recently had the opportunity to present work at the Science, Engineering and Technology for Britain exhibition at the House of Commons in London and EuroScience Open Forum in Turin, Italy.

## **High Pressure: A Trigger for Biomolecular Transformations**

*Nicholas Brooks, Beatrice Gauthé, Nick Terrill, Richard Templer, Oscar Ces, John Seddon*

High pressure can be used to induce a vast range of structural changes in soft matter systems from triggering phase changes in model membranes to causing proteins to unfold, in fact any change that involves a volume reduction can be promoted with pressure. As well as broad applicability, pressure changes can be applied very quickly and equally fast both up and down, in contrast to other structure change triggers such as temperature jumps. Fast jumps in pressure (around 5 ms) allow the trigger to be decoupled from any structural change and so with a fast structure probe such as time resolved X-ray diffraction, the out of equilibrium evolution of these systems can be monitored. Despite the great advantages over other structural change initiators, high pressure remains underutilised primarily due to its technical challenges.

We have developed a pressure-jump system for small and wide angle X-ray diffraction, which is designed to open this highly advantageous technique to a broad user base. The system is stationed at beamline I22, Diamond Light Source, UK and is freely available to beamline users. The pressure cell is highly robust requiring virtually no user intervention during an experiment beyond sample changing, and the pressure system is remotely controlled via a graphical user interface. Pressures between 0 and 500 MPa are available and jumps within this range can be carried out in approximately 5 ms at temperatures from -10 to 120°C. Both pressure jumps and static pressure – temperature scans can be set up and run automatically, significantly improving sample throughput and reducing user contact time. The system has been designed to allow studies of a broad range of samples including liquid crystals and protein solutions. Sample changing has been made as simple and fast as possible with a dedicated sample loading port and modular sample holders.





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Thomas Huddle joined the University of Nottingham in 2004 to undertake a MSci Chemistry course. The third year of this undergraduate course was spent on exchange at the University of New South Wales in Sydney, Australia. Research at UNSW included the development of transparent super-hydrophobic surfaces with the application of anti-fouling of naval vessels. His fourth year masters project at the University of Nottingham concerned the hydrothermal synthesis of nanoparticles in supercritical water; this project was conducted under the supervision of Prof. Martyn Poliakoff in collaboration with the chemical engineering department. Following graduation in 2008, Thomas has continued work within Martyn's research group as a PhD student working on a CASE project in collaboration with Lucite International, the world's leading supplier of Methyl Methacrylate. His PhD research investigates alternative methods of generating acrylic monomers from biomass, rather than petrochemical precursors. During his studies, Thomas has also developed a business venture in graphic design and animation, primarily targeted at the scientific academic and industrial communities. This business has provided high-end animation solutions for the marketing of scientific intellectual property developed within the University of Nottingham, as well as for the education sector. Graphical works have also been featured as journal covers of "Chemical Communications" and "Chemical Reviews".

**Name:** Thomas Andrew Huddle

**Project Title:** The Generation of Acrylic Monomers from Renewable Feedstocks  
(Collaborative project between University of Nottingham and Lucite International)

**Stage of Career:** PhD Student, Year 2

**Supervisor:** Professor Martyn Poliakoff

**Abstract:**

Lucite International is the world's leading supplier of Methyl Methacrylate (MMA), producing over 1.1 megatonnes per year. Currently MMA is produced via the conventional Acetone Cyanohydrin (ACH) route, as well as Lucite's new "Alpha Process" method. Although Lucite's Alpha Process presents numerous advantages to the traditional ACH route, regarding both efficiency and safety, all current processes used in the production of MMA ultimately rely on the use of petrochemical feedstocks.

There is no direct biological pathway to convert biomass into MMA or Methacrylic Acid. It has been shown that certain acids, such as Citric and Itaconic Acids, may undergo decomposition via oxidative decarboxylation in water at elevated temperature and pressure, to yield Methacrylic Acid. Such acids may be produced from fermentation of sugars, in the presence of the appropriate enzymes. Methacrylic Acid is easily converted to Methyl Methacrylate via esterification.

Essentially, it may be possible to generate Methacrylic Acid from biomass using a tandem fermentation/hydrothermal decomposition process, should the yields, selectivity and energy efficiency be optimised to an extent where the process is economically viable. Such a process would eliminate the requirement of petrochemical feedstocks in the generation of a primary building block used in the plastics industry.

Although the formation of Methacrylic Acid via the decarboxylation of renewable acids is known to occur, there are a large number of factors affecting the selectivity and yield in such a process. Numerous parasitic reactions are possible, some of which are irreversible, thus impairing the efficiency of the process. Methacrylic Acid itself is also susceptible to degradation at elevated temperature and pressure and is also vulnerable to attack from other by-products produced in the process. Appropriate catalysts and conditions may improve selectivity to the desired process and may reduce the severity of conditions required, hence minimising decomposition of the Methacrylic Acid produced. For the process to be economically feasible, a substantially high selectivity and yield must be achieved through detailed understanding and precise optimisation of the relevant process conditions.