

Research in the School is divided into three research units; examples of specific research topics are given below each unit heading and unit leader. Individual staff research summaries are also listed below and more details can be found on the School of Chemistry website:

<http://www.birmingham.ac.uk/schools/chemistry/index.aspx>

Materials Chemistry

Unit Leader: Prof. Peter Slater

Biotemplating; biologically switchable surfaces; computer modelling of materials; drug delivery and the development of novel antimicrobials; encapsulation of small molecules; ferroelectrics; functional materials; gene delivery; green synthesis; heterogeneous catalysis; high-pressure chemistry; hybrid organic-inorganic materials; hydrogen storage and separation; fuel cell/electrolyser materials; Li/Na ion battery materials including recycling; magnetic materials; metal organic frameworks; nanoparticles, nanowires and micelles; organic materials; polymers; polymorphism; self-assembly; sensing and imaging; structural chemistry; thermoelectric materials; nuclear waste encapsulation materials; zeolites.

Interactions, Interfaces and Sensing

Unit Leader: Prof. Roy Johnston

Analytical science; bio-nanotechnology; biophysical chemistry; catalysis; charge transfer and transport; clusters and nanoparticles; electrochemistry; environmental chemistry; fluorescence; magnetic resonance spectroscopy and imaging; optical sensors; scanning probe microscopy; self-assembly; simulation and modelling; single molecule imaging; soft matter; solvation effects; surface and interfacial chemistry; synchrotron-based characterisation; theoretical chemistry.

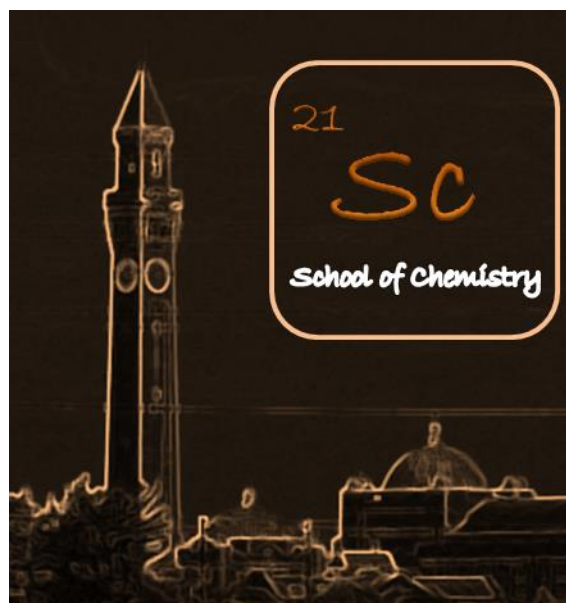
Synthesis, Biological and Supramolecular Chemistry

Unit Leader: Prof. Andrew Dove

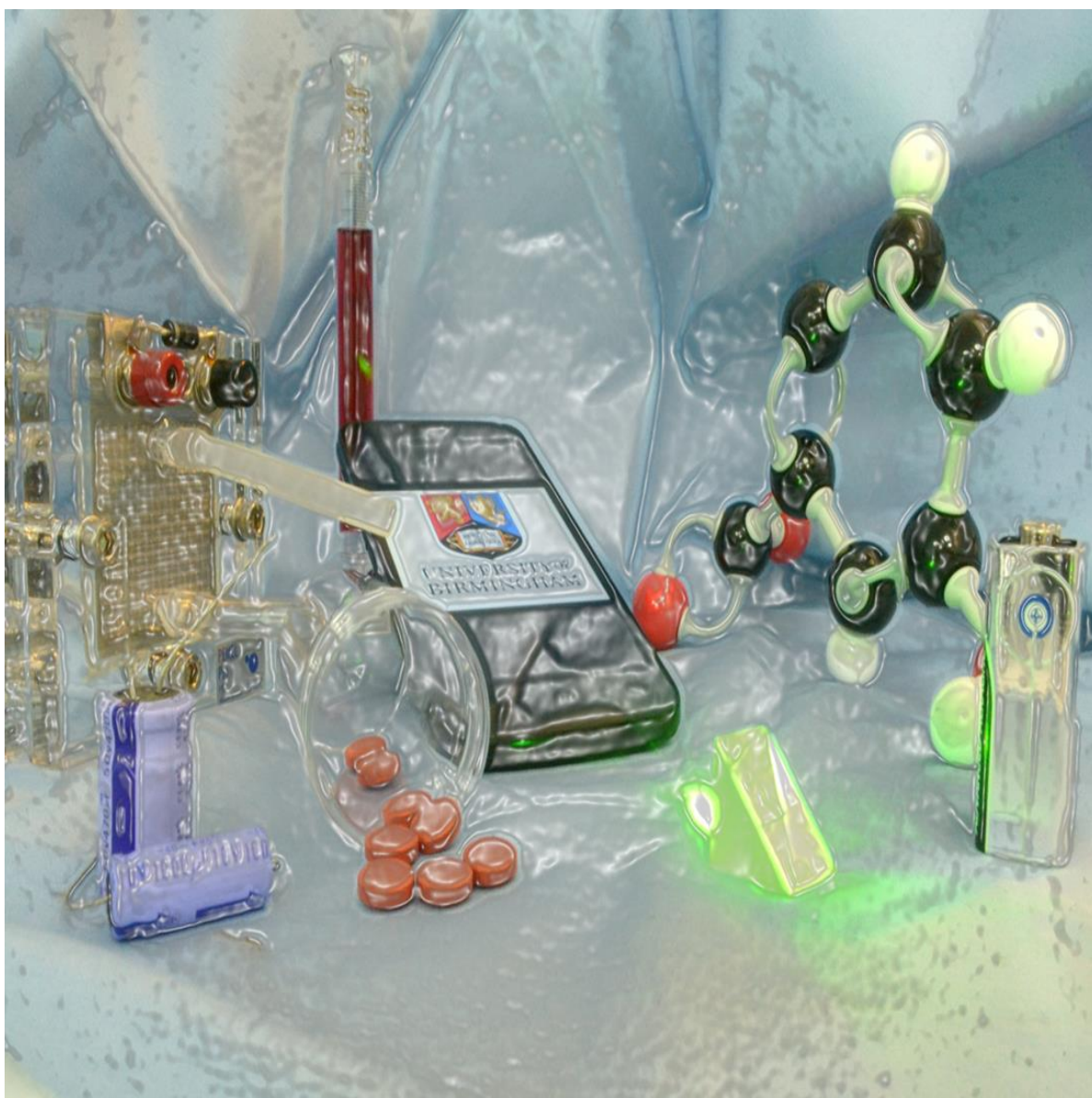
Asymmetric synthesis and catalysis; peptides, carbohydrates and lipids; molecular design and diversity; synthetic organic and inorganic chemistry; sustainable chemistry; molecular and biomolecular recognition; supramolecular architectures; bioinorganic systems; photophysics and photochemistry; DNA recognition motifs; metallo-drugs and imaging agents.



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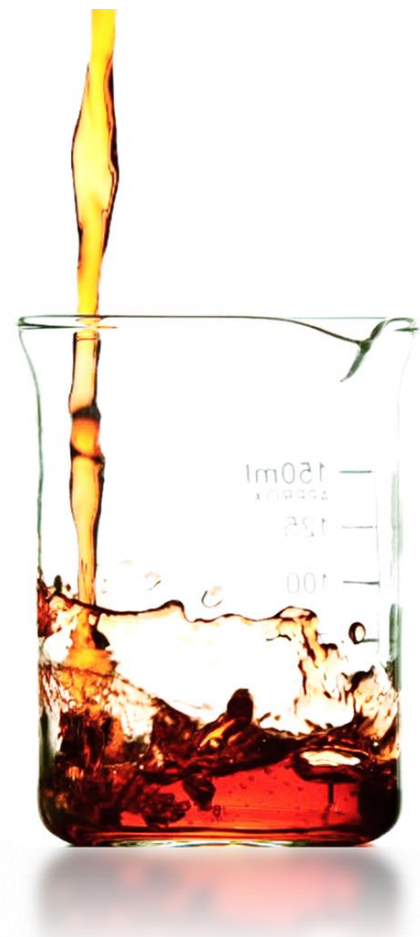


RESEARCH OPPORTUNITIES
IN THE SCHOOL OF
CHEMISTRY



The School of Chemistry has undertaken world-leading research for over a century and remains at the forefront of scientific discovery, as recently recognised in the 2014 Research Excellence Framework (REF2014), where all of our research outputs were graded as internationally recognised, with over 95% being classed as internationally excellent or world-leading.

In addition to work in the four research units described here, the School also has three outward facing research themes that reflect the cross-disciplinary nature of the research that we undertake. More details of these can be found here: <http://www.birmingham.ac.uk/research/activity/chemistry/research-themes/index.aspx>



Postgraduate Opportunities

Each year, we have approximately 20 PhD postgraduate scholarships available to UK/EU students. Applicants should have, or expect to obtain, a first- or upper second-class Honours MSci/MChem degree, or the equivalent, in Chemistry or a relevant related discipline.

International (non EU) students can often be funded through overseas research scholarships, Commonwealth scholarships or their home government. International students with their own scholarships are welcome to apply, but should ensure that sponsors make allowance for the payment of University and bench fees as well as living costs in their award.

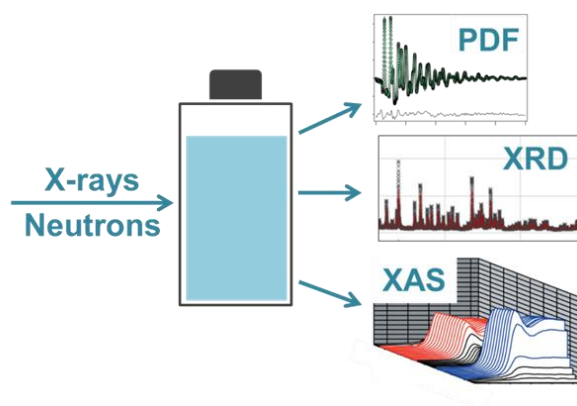
- EPSRC industrial CASE awards may attract a financial contribution from the industrial sponsor; fully-funded industrially-sponsored scholarships are also usually available on terms comparable with EPSRC grants, including payment of fees.

For further information on our postgraduate opportunities, please email: chemistry-pgadmissions@contacts.bham.ac.uk

Fellowship Opportunities

We welcome enquiries over postdoctoral positions and from researchers wishing to start their independent academic career through a fellowship (e.g. EPSRC, Royal Society). Postdoc applicants should contact staff members directly, whereas potential fellowship holders should contact Prof. Tim Albrecht, the School's Director of Research, t.albrecht@bham.ac.uk

Materials Chemistry



DR. PHOEBE ALLAN

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My research focus is materials chemistry for energy storage. I aim to understand the links between the structure of a material and its physical properties using techniques including synchrotron X-ray and neutron powder diffraction, pair distribution function (PDF) analysis and spectroscopic techniques (Raman, NMR, X-ray adsorption spectroscopy (XAS)). A particular interest is developing experiments which allow us to probe the structure of a material as it changes, in real-time and under operational conditions. This approach informs us which structural features are desirable for obtaining new materials with improved performance allowing the rational design of optimised materials. Current areas of interest include new electrode and electrolyte materials for lithium- and sodium-ion batteries.

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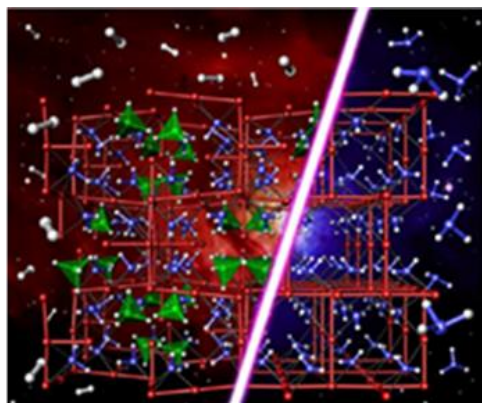
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Exfoliation of layered Na-ion anode material $\text{Na}_2\text{Ti}_3\text{O}_7$ for enhanced capacity and cyclability, M. A. Tsiamtouri, P. K. Allan, A. J. Pell, G., Kim, R. N. Kerber, P. C. M. M. Magusin, D. A. Jefferson, C. P. Grey, *Chemistry of Materials*, **2018**, 30, 1505

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DR. PAUL ANDERSON

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The primary aims of my research are the discovery and characterization of new inorganic materials (many of which have potential applications related to energy) and the development of new recycling processes. Important research areas: development of efficient and economic processes for the recycling of automotive lithium ion batteries; synthesis of new potential hydrogen storage materials for use in safe hydrogen delivery systems or reversible hydrogen stores; synthesis of new ion-exchangeable metal-organic framework materials (MOFs); development of new applications for zeolite and MOFs in adsorption cooling, desalination and environmental remediation; synthesis of new solid state electrolytes for lithium and sodium ion batteries.

Web: www.birmingham.ac.uk/staff/profiles/chemistry/anderson-paul.aspx

<https://faraday.ac.uk/recycle-reuse/>

www.birmingham.ac.uk/research/activity/energy/research/centre-strategic-elements-critical-materials/index.aspx

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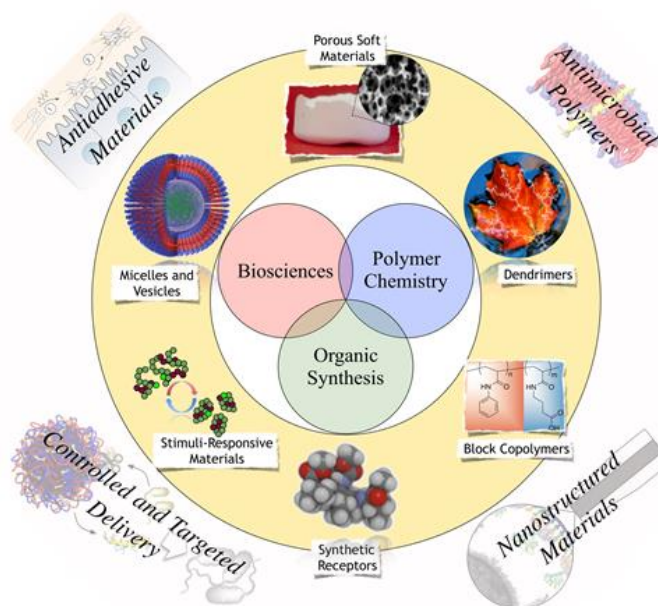
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DR. FRANCISCO FERNANDEZ-TRILLO

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Our research lies at the interface between Organic Chemistry, Polymer Science and Life Sciences. We aim to develop well-defined multivalent materials that can work at the nanoscale. Control over degree and type of functionality, size and architecture are key goals in the development of functional materials that act as tools in Biology and Medicine. Key applications include sensing and imaging, drug delivery or the development of novel antimicrobials.



Web: <http://www.birmingham.ac.uk/staff/profiles/chemistry/fernandez-trillo-francisco.aspx>

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Engineering microbial physiology with synthetic polymers: cationic polymers induce biofilm formation in *Vibrio cholerae* and downregulate the expression of virulence genes. N. Perez-Soto, L. Moule, D. N. Crisan, I. Insua, L. M. Taylor-Smith, K. Voelz, F. Fernandez-Trillo and A. M. Krachler, *Chem. Sci.*, **2017**, 8, 5291.

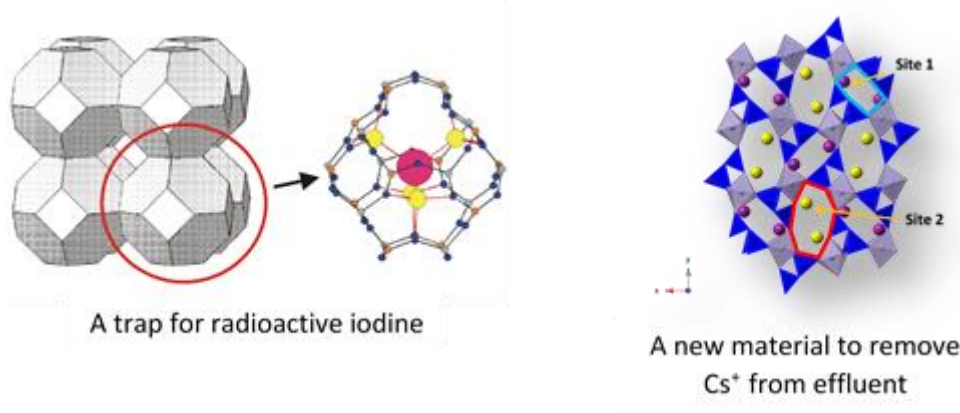
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DR. JOSEPH HRILJAC

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Our research focusses on inorganic solids that are porous at the molecular scale, such as aluminosilicate zeolites and tetrahedral-octahedral materials such as tin silicates with the umbite structure. We synthesise and characterise new materials for a wide range of applications but of late this has principally been for environmental remediation of legacy nuclear waste including the transformation of porous solids into wasteforms for long-term storage. This has included involvement in the large multi-University consortia DISTINCTIVE (Decommissioning, Immobilisation and Storage Solutions for Nuclear Waste Inventories) and TRANSCEND (Transformative Science and Engineering for Nuclear Decommissioning). We work closely with both University and Industry partners. Much of the characterisation focusses on developing structure-property relationships and analysis using crystallographic techniques, especially X-ray (conventional and synchrotron) and neutron powder diffraction or total scattering studies using Pair Distribution Function analysis at ambient or non-ambient temperatures or pressure.



Web: www.birmingham.ac.uk/staff/profiles/chemistry/hriljac-joseph.aspx

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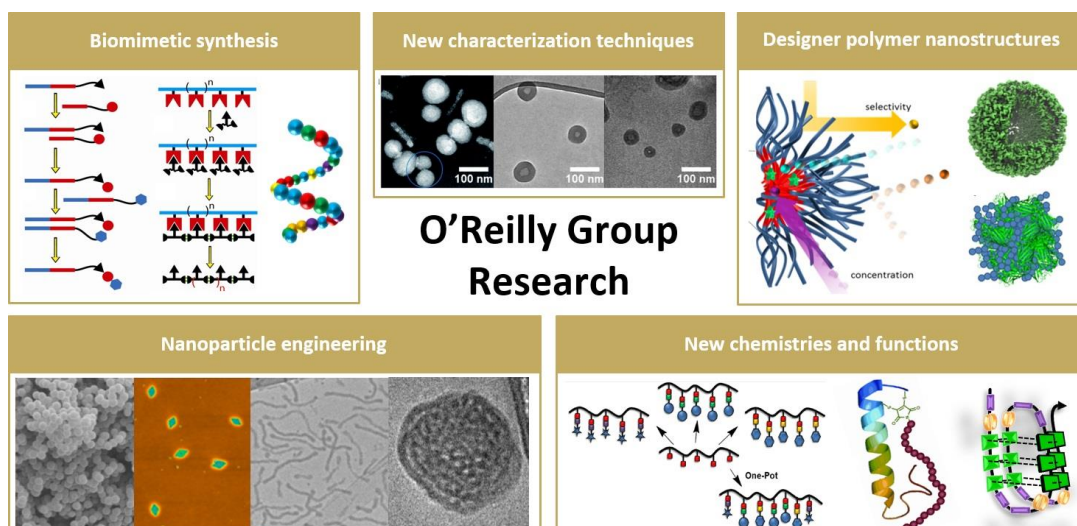
Ammonia removal from water using sodium hydroxide modified zeolite mordenite, J. P. Soetardji, J. C. Claudia, Y.-H. Ju, J. A. Hriljac, T.-Y. Chen, .F. E. Soetaredjo, S. P. Santoso, A. Kurniawan and S. Ismadji, *RSC Advances* **2015**, 5, 83689.

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PROF. RACHEL O'REILLY
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Our research targets the design, synthesis and application of uniquely derived polymeric materials; where control over architecture, functionality and reactivity are central to their application in the field of nanotechnology. We are especially concerned with the synthesis of polymeric materials using both established chemistries and developing new synthetic polymerisation strategies. The supramolecular assembly of these polymers into precision nanostructures, such as organic/inorganic or hybrid nanoparticles is of interest given their ability to mimic biomolecules in size, structure and function and also possess novel properties, including the ability to behave as hosts or vessels in delivery agents. The subsequent assembly of these nanoparticles in one-, two- and three dimensions, and their chemical modification, can be applied to afford materials with potential applications as biological mimics, nanoreactors and nanotechnology devices.

The core of our research is in the area of polymer synthesis and involves the development of controlled radical polymerization chemistries (in particular reversible addition fragmentation chain transfer or RAFT techniques) for the synthesis of well-defined and functional macromolecules. My group are especially focused on the design and synthesis of materials that enable supramolecular assembly to form precision hybrid nanostructures with a specific focus on micellar structures, responsive materials and crystallization driven assembly. We also work at the biology-materials interface and have an interest in DNA templating chemistries, protein conjugation and sequence controlled materials.



Web:

<http://www.birmingham.ac.uk/schools/chemistry/people/navigation.aspx?ReferenceId=137738&Name=professor-rachel-o%27reilly>

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One-pot synthesis of super-bright fluorescent nanogel contrast agents containing a dithiomaleimide fluorophore. M.P. Robin, J.E. Raymond and R.K. O'Reilly. *Materials Horizons*, **2015**, 2, 54.

Dispersity Effects in Polymer Self-Assemblies: A Matter of Hierarchical Control, K. E. B. Doncom, L. D. Blackman, D. B. Wright, M. I. Gibson, and R. K. O'Reilly, *Chem. Soc. Rev.* **2017**, 46, 4119.

PROF. JON PREECE

Email: j.a.preece@bham.ac.uk

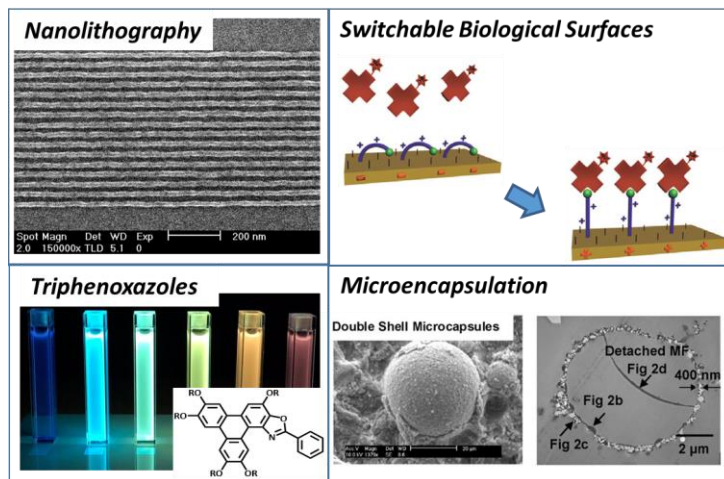
The Preece Group has interests in:

a. Nanofabrication: Nanofabrication is a key technology in many high technology sectors including the electronics, medical and sensor industries. Fabrication of chemically patterned substrates on the nanoscale requires lithographic techniques with nanometer resolution, as well as materials that allow a controlled modification of their properties. Thus, the Preece group in collaboration with the Robinson group (Chem Eng) carries out research in the area of chemically-nanopatterning thin films using e-beams and E-UV sources, which has led to the founding of a university spin out company – Irresistible Materials Ltd (irresistiblematerials.com).

b. Biologically switchable surfaces: The ability to control the binding of bioactive molecules to a surface is technologically important as it potentially allows control of fouling of surfaces, sensing, and delivery of drugs, for example. In collaboration with the Mendes Group (Chem Eng) we have designed a system in which a molecular structure can be controlled by applying a potential to a surface, which in turn controls the rate of binding.

c. Advanced Organic Electronic Materials: The Preece group have discovered a new class of organic material – the Triphenoxazoles – which when photoexcited can (a) fluoresce blue through to red, displaying the largest Stoke shift of any purely organic material, and (b) generate a photocurrent which is 50 times larger than the parent triphenylene structure (a known good material for supporting photocurrent) from which they are derived, and (c) support a liquid crystalline mesophase. Thus, these materials have potential technological applications as organic photovoltaics and light emitting diodes.

d. Formulation Engineering and Encapsulation of Small Molecules: In collaboration with the Zhang group (Chem Eng) and industry we have designed several systems in which small molecules are encapsulated with a micron scale capsule. These capsules modulate the release profiles of the molecules both through chemical and mechanical means. These materials have applications ranging from drug delivery to personal care products, such as shampoo.



Web: www.birmingham.ac.uk/staff/profiles/chemistry/preece-jon.aspx

Controlling Gold Nanoparticle Assembly on Electron Beam-Reduced Nitrophenyl Self-Assembled Monolayers via Electron Dose. S.J. Leigh, J.L. Prieto, J. Bowen, S. Lewis, A.P.G. Robinson, P. Iqbal, J.A. Preece, *Colloids and Surfaces A – Physicochemical and Engineering Aspects*, **2013**, 433, 181.

‘Electrically Responsive Surfaces: Experimental and Theoretical Investigations. E. Cantini, X. Wang, P. Koelsch, J.A. Preece, J. Ma, P.M. Mendes, *Acc. Chem. Res.*, **2016**, 49, 1223.

A Brief Review of Carbazole-Based Photorefractive Liquid Crystalline Materials. M. Manickam, P. Iqbal, M. Belloni, S. Kumar, J.A. Preece, *Israel Journal of Chemistry*, **2012**, 52, 917-934

The First Example of Sustained Release of a Water Soluble Inorganic Salt from Novel Polystyrene Sulfonate-Silica Microspheres via Dual-Release Mechanism C. Sui, J.A. Preece, Z. Zhang, *RSC Advances*, **2017**, 7, 478.

DR. MARK S D READ

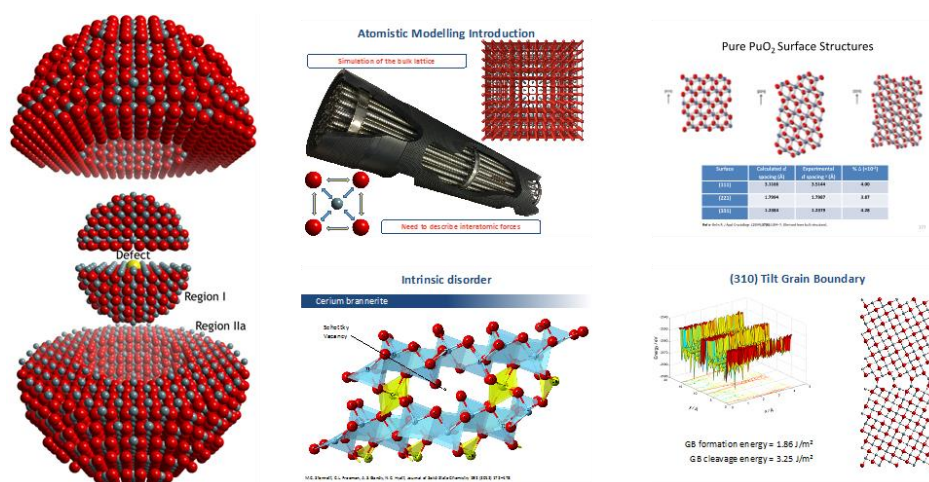
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Our research targets a range of topics within contemporary materials chemistry modelling, with particular focus on the deployment and development of atomistic simulation methodologies to extend our understanding of the structure, stability and reactivity of solid state materials at the atomic level, particularly those with relevance to industrial and energy applications. The main focus of our research lies in civil nuclear fuels (actinide oxides), the ageing concerns with the storage of special nuclear materials and candidate matrices for high level waste encapsulation. Ageing, performance and mechanical properties are predicted through static and molecular dynamic approaches to simulating radiation damage and defect chemistries of the materials.

Civil nuclear fuels: Current activity includes the simulation of ageing effects on nuclear fuels (uranium, plutonium, thorium and 'mixed' oxides), radiation damage and modelling the defect chemistry within the bulk and at surfaces (which control many important material properties). Indeed, the corrosion of nuclear fuels is an extremely pertinent area of research and is crucial to the safety and sustainability of the nuclear fuel cycle.

Candidate matrices for high level waste encapsulation: Nuclear energy research in the UK is currently undergoing a renaissance due to the need to reduce the reliance on carbon-based fuels and to meet the country's long term CO₂ emission reduction commitments. New reactors are planned to replace existing plant but there is considerable public scepticism especially concerning safety and waste storage. It is thus important to demonstrate the effectiveness of current waste storage methods when products remain active over many years and to develop improved methods.

Storage of Special Nuclear Materials: Work focuses on enhancing the understanding of PuO₂ properties and behaviour relevant to storage scenarios. Using a classical potential approach, a variety of purpose-built codes have been used to model properties of the bulk material, surfaces and defects including helium. We are interested in the investigation of He trapping sites and accumulation in Schottky voids/grain boundaries, predicting He behaviour and effects on PuO₂ lattice and surfaces, the effect of radiation damage on mobility of defects and ageing mechanisms, the ageing defect chemistry under a variety of stoichiometries (e.g. Am ingrowth) and effects on surface chemistry of extrinsic defects



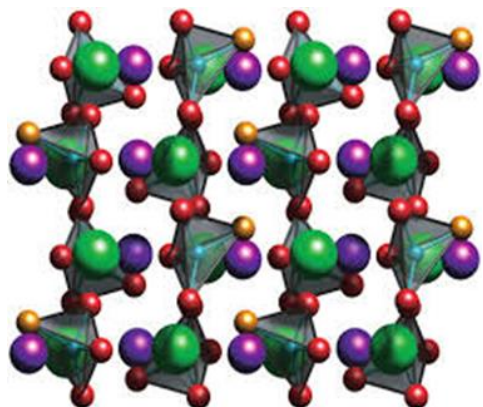
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Activity computer program for calculating ion irradiation activation. B. Palmer, B. Connolly, and M. S. D. Read. *Computer Physics Communications*, **2017**, 216, 138.

Derivation of enhanced potentials for cerium brannerite and the calculation of lattice and intrinsic defect properties. R. A. Bird and M. S. D. Read. *Nuclear Instr. & Methods in Phys. Res. Section B-Beam Interactions with Mat. and Atoms*, **2017**, 393, 63.

Derivation of enhanced potentials for plutonium dioxide and the Calculation of lattice and intrinsic defect properties. M. S. D. Read, S. R. Walker and R. A. Jackson. *Journal of Nuclear Materials*, **2014**, 448, 20.



PROF. PETER SLATER

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My research is in the area of materials chemistry, with the main focus on the development of new materials for energy applications. This includes the investigation of novel materials for use in Solid Oxide Fuel Cells and solid state Li ion batteries. This research has led to the identification of new structure-types displaying ionic conductivity, as well as new doping strategies to improve the performance of existing materials. My research group also has interests in the synthesis and characterisation of mixed metal oxide fluorides prepared by low temperature routes for a range of applications. Experimental techniques employed include X-ray and neutron diffraction, conductivity measurements, thermogravimetric analysis, Raman and NMR spectroscopy.

Web: www.birmingham.ac.uk/staff/profiles/chemistry/slater-peterraymond.aspx

Investigation into the dehydration of selenate doped $\text{Na}_2\text{M}(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$ ($\text{M} = \text{Mn, Fe, Co and Ni}$): stabilisation of the high Na content alluaudite phases $\text{Na}_3\text{M}_{1.5}(\text{SO}_4)_{3-1.5x}(\text{SeO}_4)_{1.5x}$ ($\text{M} = \text{Mn, Co and Ni}$) through selenate incorporation; L.L. Driscoll, E. Kendrick, K.S. Knight, A. J. Wright and P.R. Slater; *Solid State Chem* **2018**, 258, 64.

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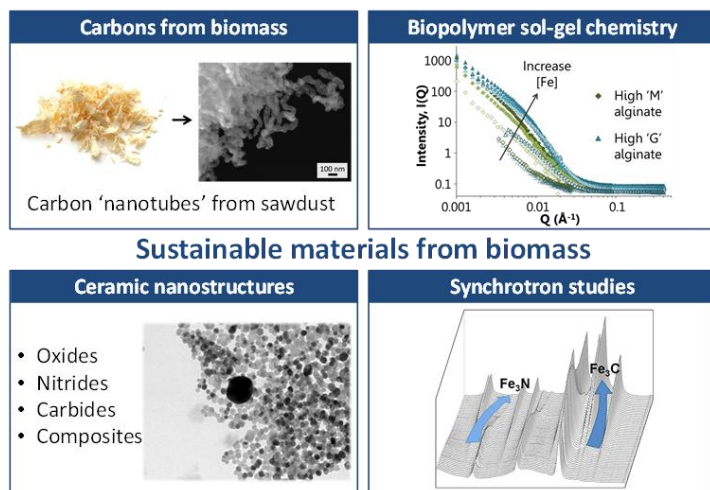
Synthesis, structural characterisation and proton conduction of two new hydrated phases of barium ferrite $\text{BaFeO}_{2.5-x}(\text{OH})_{2x}$; P. L. Knöchel, P.J. Keenan, C. Loho, C.Reitz, R. Witte, K. S. Knight, A.J. Wright, H. Hahn, P. R. Slater, O.Clemens; *J. Mater Chem. A* **2016**, 4, 3415.

DR. ZOE SCHNEPP

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Our research targets the sustainable synthesis of materials from nanostructured carbons to ceramics and composites. We are particularly interested in the use of biomass as a precursor for materials synthesis, including raw biomass sources such as agricultural waste and pure biological polymers (biopolymers). The diverse structures and chemistries of biological materials offer us unprecedented control over the structure and functionality of ceramic and carbon materials.

A core of our research is focussed on understanding how biological materials are able to control the formation of unique nanostructures of ceramics and carbons. Our group uses and develops advanced synchrotron, neutron and electron microscopy techniques to study all stages of materials synthesis, from the structure of biopolymer sol-gel precursors to the high temperature graphitization of biomass.



Web: www.schneppgroup.wordpress.com

<http://www.birmingham.ac.uk/schools/chemistry/people/navigation.aspx?ReferenceId=49314&Name=dr-zoe-schnepp>

Mechanistic insights into the formation of porous carbons from gelatin, A. E. Danks, M. J. Hollamby, B. Hammouda, D. C. Fletcher, F. Johnston-Banks, S. E. Rogers, Z. Schnepp, *J. Mater. Chem. A*, **2017**, 5, 11644.

The evolution of 'sol-gel' chemistry as a technique for materials synthesis, A. E. Danks, S. R. Hall, Z. Schnepp, *Mater. Horiz.*, **2016**, 3, 91.

In situ synchrotron X-ray diffraction study of the sol-gel synthesis of Fe_3N and Fe_3C , Z. Schnepp, A. E. Danks, M. J. Hollamby, B. R. Pauw, C. A. Murray, C. C. Tang, *Chem. Mater.*, **2015**, 27, 5094.

Iron catalyzed graphitization of biomass, E. Thompson, A. Danks, L. Bourgeois, Z. Schnepp, *Green Chemistry*, **2015**, 17, 551.

Interactions, Interfaces and Sensing

PROF. TIM ALBRECHT

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Our research interests revolve around charged interfaces and charge transport at the nanoscale and in electrochemical environments.

Charge Transport in Single Molecules: While charge transport in linear molecules is fairly well understood, the situation is quite different for branched or ring-shaped molecules. Depending on the charge transport mechanism, quantum interference (QI) or new types of hopping phenomena may occur, which in the case of QI can enhance the thermoelectric performance of a molecule. Hence, in this activity we study 'new' molecules, in an effort to understand their complex interfacial and charge transport behaviour.

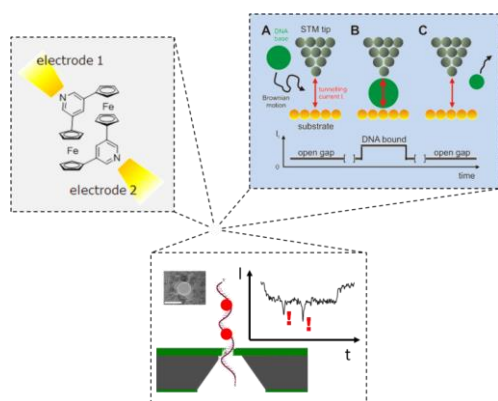
Quantum Tunnelling for Sensing and Sequencing: Is it possible to use the quantum-mechanical tunnelling effect for sequencing of biopolymers, such as DNA, RNA and proteins? This is an intriguing possibility, but also an enormous challenge. In recent years, we have made significant progress towards this goal, by showing that tunnelling detection of single DNA molecules is indeed compatible with a high-throughput analysis platform (nanopores). Now we are pushing the limits on single-base detection in EC-STM, with a combination of surface engineering and state-of-the-art machine learning techniques, inc. Deep Learning (see below).

Single-molecule sensing with nanopore and nanopipettes: This is an exciting field of research, which spans from fundamental biophysical studies on biopolymers to biosensing and diagnostics. Based on rather unique instrumental capabilities, we are in a position to not only detect and control translocation of single biomolecules, but also to characterize them at a sub-molecular level. This opens up new avenues towards all-electronic biosensing and new types of DNA assays.

Machine Learning in Single-Molecule Science: The exploration and application of Machine Learning tools has become an underpinning theme in various aspects of our work, including dimensionality reduction techniques (PCA, MPVC, t-SNE), Autoencoders for unsupervised classification, Support Vector Machines, and Deep Learning methods such as Convolutional Neural Networks.

Web:

<http://www.birmingham.ac.uk/schools/chemistry/people/navigation.aspx?Referenceld=134956&Name=professor-tim-albrecht>



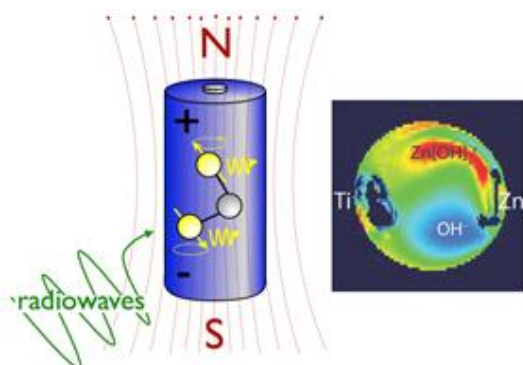
Ferrocene- and Biferrocene-Containing Macrocycles towards Single-Molecule Electronics. LE Wilson, C Hassenr ck, RF Winter, AJP White, T Albrecht, NJ Long. *Angew. Chem. Int. Ed.*, **2017**, 56, 6838.

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Magnetic resonance imaging (MRI) visualisation of battery chemistry.

DR. MELANIE BRITTON

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The Britton group is a leader in developing Nuclear Magnetic Resonance (NMR) spectroscopy and imaging (MRI) methods to probe chemical composition and processes in materials important in energy storage, nanoparticle synthesis and consumer products. NMR measurements of diffusion are employed to characterise the structure, shape and exchange properties of micelles, reverse micelles and vesicles in a variety of surfactant systems, which has provided insight into how these complex media are able to support chemical reactions and, in collaboration with industry, improve product stability in detergents and other important consumer products. We use MRI to visualise chemical reactions; develop contrast agents in biomedical applications; and visualise battery chemistry. Using MRI, we can visualise flow and better understand how chemistry couples with flow during chemical and biological pattern formation, as well as in chemical reactors. We have shown that MRI can be used to probe the composition and structural changes in an electrolyte solution by a reactive metal during corrosion. Recently, we have extended this research to visualise the electrochemistry and molecular transport inside a zinc-air and sodium-ion batteries. These novel experiments demonstrate the enormous potential for MRI to study a range of electrochemical systems such as energy storage, corrosion prevention and electroplating.

Web:

www.birmingham.ac.uk/staff/profiles/chemistry/britton-melanie.aspx

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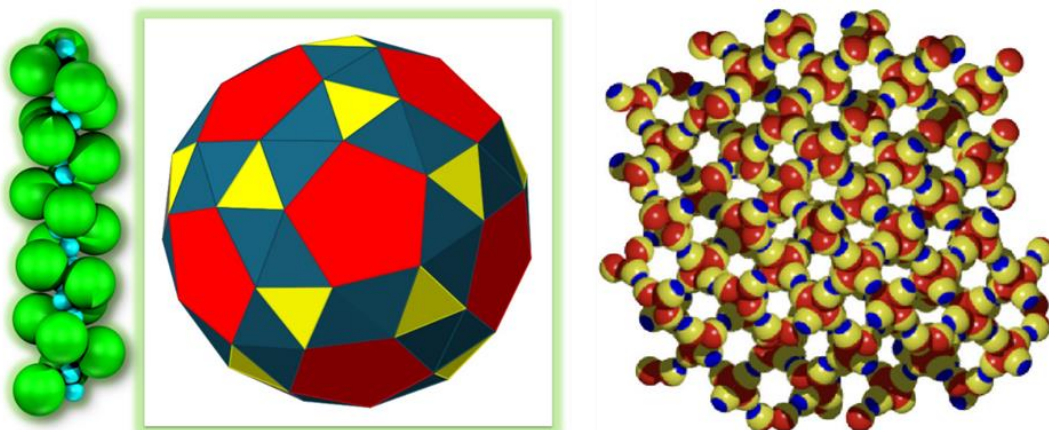
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DR. DWAIPAYAN CHAKRABARTI

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The overarching theme of our research is in silico design of soft materials, including biomaterials, to inform fabrication of functional architectures as well as formulation of consumer products. The study of soft matter is central to this research theme. We are particularly interested in designing bottom-up routes to novel photonic, porous, responsive and viscoelastic materials. We consider a range of building blocks, from molecular to microscale, for their programmed self-assembly. Our recent focus has been on programming hierarchical self-assembly of colloidal particles, thus addressing a multiscale design problem.

Active colloids are microscale particles, which self-propel through viscous fluids by transducing energy into mechanical work and thus mimic the self-propulsion of living organisms. Active colloids, and more generally active matter, are at the forefront of current soft matter research with rich non-equilibrium phenomena. We are also studying structural and dynamic properties of active colloidal suspensions, especially in the context of emergent collective behaviour, in order to programme self-organisation of active colloids. To this end our research develops, adapts, and applies computational methods, largely underpinned by the theory of statistical mechanics and energy landscape framework, to study systems of interest in close connection with contemporary experimental research.

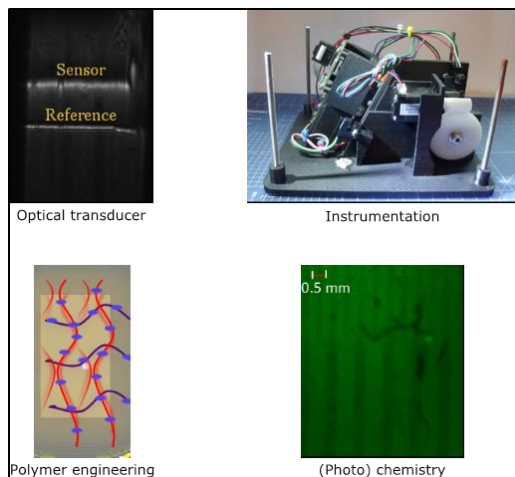


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DR. RUCHI GUPTA

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The research theme in Gupta group is polymeric optical sensors. Polymers offer chemical diversity that allow us to tailor their physiochemical properties. We design internally referenced transducers and associated instrumentation to analyse species of interest in "real" samples and environmental conditions. A significant activity in the group is also focused on polymer engineering and their characterisation. Additionally, we are developing chemistries for the fabrication of an array of sensors using solution processing methods in a single step. We collaborate with researchers in clinical sciences and industry to exploit the application of our sensors in point-of-care/ point-of-use analysis.

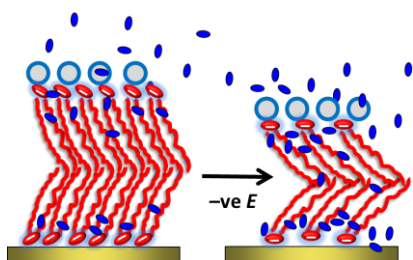
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<http://www.birmingham.ac.uk/schools/chemistry/people/navigation.aspx?Referenceld=126213&Name=dr-ruchi-gupta>

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DR. SARAH HORSWELL

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Application of in situ infrared spectroscopy to study molecular adsorption at solid metal electrodes. Of current interest is the effect of electric potential on molecular conformation of phospholipids assembled on gold surfaces. These assemblies mimic cell membranes and can be used to bind other biological molecules to the surface. This provides opportunities to tailor surfaces at the nanometre scale and has potential application in the manufacture of biosensors. Our other main interest is the synthesis and electrochemical properties of bimetallic nanoparticles. The nanoparticles are tethered to substrates and their catalytic activity towards electrochemical reduction reactions is determined.

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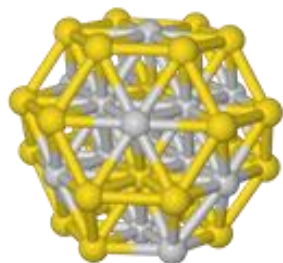
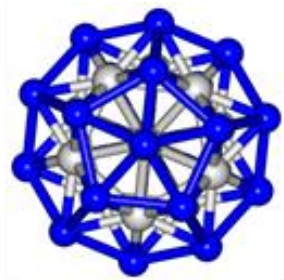
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PROF. ROY JOHNSTON

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Theoretical/computational chemistry. A major strand of our research involves the application of biologically-inspired computational methods (particularly genetic algorithms) to chemical problems (e.g. cluster geometry optimisation and protein folding). Another important research area is the study of the structures, growth, dynamics and the chemical and physical properties of free and supported metal nanoparticles and bimetallic nanoalloys, using Density Functional Theory calculations. We also study the conformational energy landscapes and self-assembly of proteins and cyclic peptides and the solvation of polyatomic ions in water nanodroplets. We collaborate closely with experimental research groups in Chemistry and Physics, within the University, as well as nationally and internationally.

Web: www.birmingham.ac.uk/staff/profiles/chemistry/johnston-roy.aspx

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DR. ROBERT NEELY

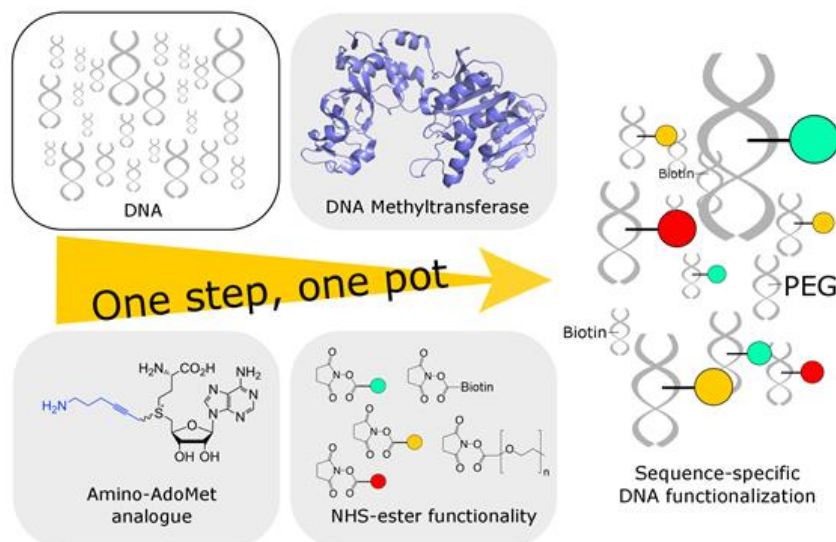
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Our research focusses on the genome; its chemistry, structure and function. Our work is interdisciplinary and combines state-of-the-art analytical approaches, such as nanopore DNA sequencing and super-resolution microscopy with novel chemical biology.

DNA Mapping: Visualization of DNA Sequence: The molecules that bind DNA generally do so in way that is sequence-dependent. Yet because the interactions between e.g. a DNA and drug or DNA and a protein are non-covalent and transient, studying these process using traditional approaches is challenging. We have developed an approach that uses DNA-binding enzymes to add fluorescent labels to the genome at specific sites. We can lay entire genomes onto a microscope slide and image these labelled 'DNA barcodes'. Current work is applying this to understand cancer biology (virus replication in cancer cells).

Sequencing the epigenome: DNA modifications, such as methylation of cytosine, are a critical aspect of gene regulation. Aberrant methylation of the genome is implicated in a host of diseases yet studying methylation of DNA is prohibitively expensive. We are developing an enzymatic approach that allows us to sort methylated- from unmethylated DNA. We are able to detect methylation using nanopore DNA sequencing and are extending this work to investigate the role of methylation in cancer.

Expanding the nucleus: We are using an approach known as 'expansion microscopy' to study the three-dimensional architecture of the genome in exquisite detail. This involves embedding fluorescently-labelled cells in a hydrogel. The labels are cross-linked to the gel then the cell is removed and the gel swollen to around 5x its original size. The result is an optically-transparent gel containing a fluorescent outline of the feature of interest. We are applying this with cancer biologists in order to study DNA repair. .



Web: <http://www.birmingham.ac.uk/staff/profiles/chemistry/neely-robert.aspx>

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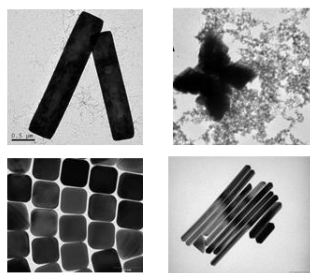
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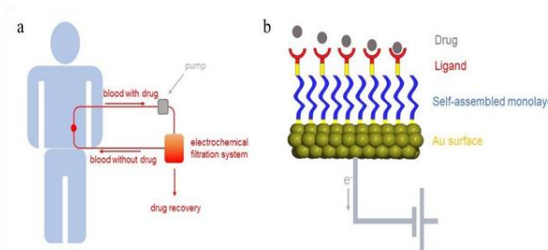
DR. PARAMACONI RODRIGUEZ
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My research is focused on the development of electrochemical technologies based on sustainable energy (re)sources, the design of new functional nanomaterials and the molecular-level understanding of electrochemical reactions in well-defined surfaces. One of the main goals of my research is to design and investigate new technologies and materials in order to improve the well-running of the Polymer Electrolyte Fuel Cell (PEFC). Other research interest includes the implementation of electrochemical methods for waste water treatment, CO₂ reduction to fuels, electrochemical nanosensor, bioelectrochemistry and chemical analysis.

Nanocatalyst Design



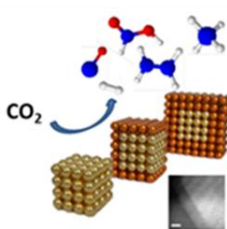
Sensing and metal recovery



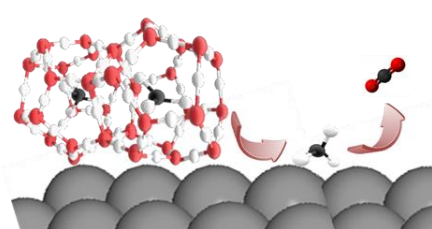
(Photo)Electrocatalysis for energy and environmental applications



Water Splitting/
Hydrogen economy



CO₂ conversion



Fuel cells and electrosynthesis

Web:

<http://www.birmingham.ac.uk/schools/chemistry/people/navigation.aspx?ReferenceId=47833&Name=dr-paramaconi-rodriquez>

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Synthesis, Biological and Supramolecular Chemistry

PROF. ANDREW DOVE

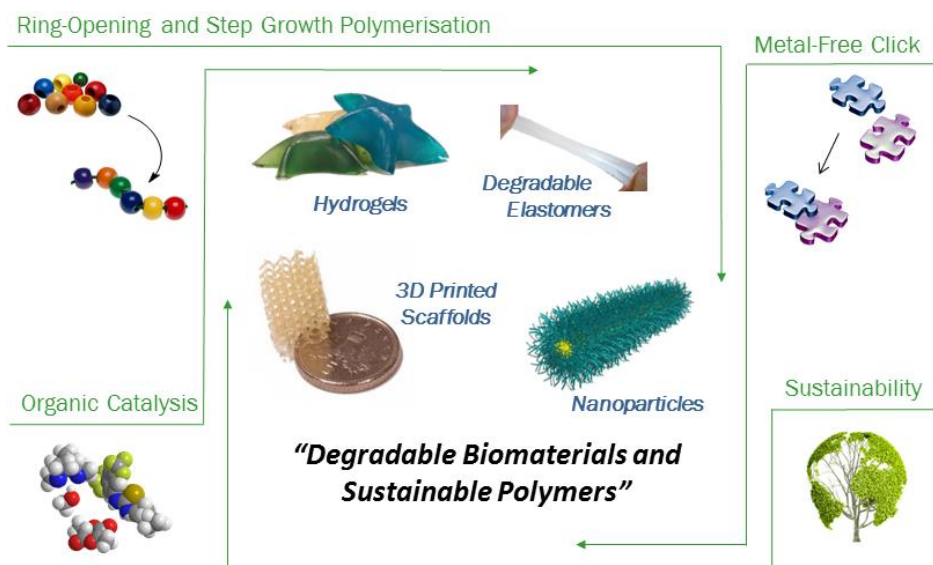
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Research in the Dove group is centered around polymer degradation. We have many strands to our research portfolio that focus on both developing strategies to control and understand polymer degradation as well as design new materials that degrade in a controlled and predictable manner. Our research efforts are in turn primarily focussed on sustainability on polymer science – that includes both ‘green’ methodologies for polymer synthesis and development of strategies to tackle plastic waste – as well as the development of next generation biomaterials – in which we seek to design materials for application in delivery and tissue engineering applications. Linking both areas is our interest in polymer stereochemistry and how that can be used to control materials properties and direct their behaviour. We work with engineers, biologists and medics across academia, hospitals and industry to drive our chemical discoveries towards application.

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<http://www.birmingham.ac.uk/schools/chemistry/people/navigation.aspx?Referenceld=137779&Name=professor-andrew-dove>

<http://dovegrouplab.com>



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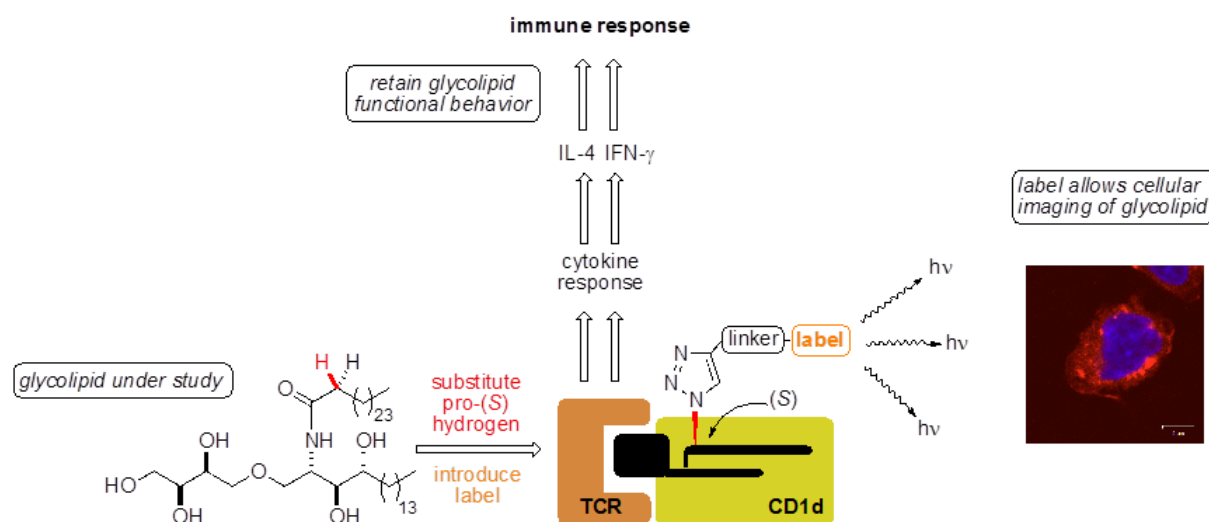
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DR. LIAM COX

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Our research spans the Chemistry–Life Sciences interface. More specifically, as synthetic chemists, we are focusing on the preparation of molecules of biological importance, working closely with Professor Del Besra in the School of Biosciences. Our research currently has two strands: in the first, we are investigating the role of glycolipids in CD1d-mediated immunity. In this project, we are not only preparing glycolipids which impart therapeutically useful immune responses, but are also developing glycolipids equipped with chemical probes to better understand their underlying biology. In a second, more medicinal chemistry-focused project, we are working closely with GlaxoSmithKline to identify and develop new drug candidates for the treatment of tuberculosis.



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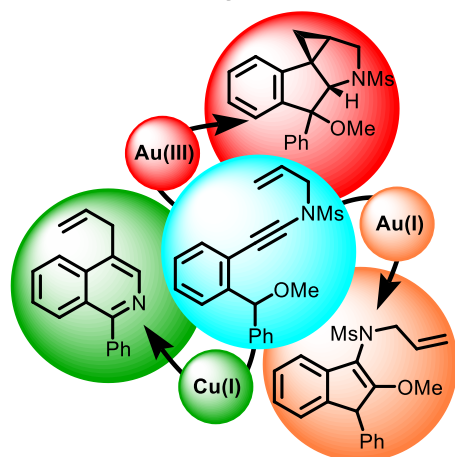
DR. PAUL DAVIES

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The Davies group's interests are mainly focused on catalysis for sustainable synthesis. Research areas include reaction discovery, transition metal chemistry, organocatalysis, ligand design and organometallic chemistry, mechanistic and labelling studies, and the target synthesis of biologically relevant products.

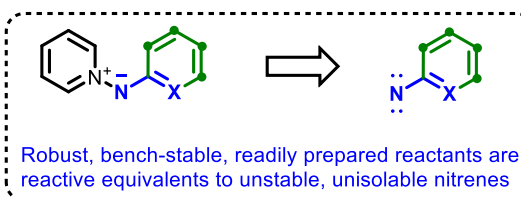
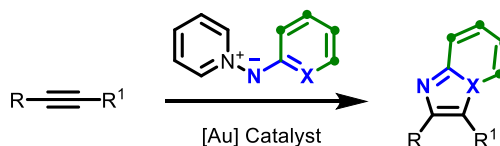
Our reaction discovery programme involves investigation-driven introduction of new modes of reactivity and catalyst design. The aim is to provide highly efficient and practical synthetic strategies alongside increasing fundamental understanding of such reactivity. Advancing these new synthetic methods provides us with convergent and general methods to rapidly access biologically relevant materials and novel functionalized scaffolds. Subsequent applications include functional motifs for catalyst design, the development of new directed fragment and scaffold libraries, and the target synthesis of biologically active molecules and mechanistic probes. Recent advances include (a) establishing ynamides as controllable metal-carbene precursors, bypassing the waste products, handling and toxicity issue associated with the use of diazo compounds; (b) establishing a novel disconnection strategy allowing functionalised azoles to be formed by formal cycloaddition.

Enabling transformations for efficient molecular synthesis using catalysis



Catalysis-controlled divergency

- Metal carbene reactivity patterns without diazocompounds
- Highly efficient, multiple bond-forming cascades
- Mild and scalable reaction conditions



New strategies for 'impossible' heterocycles

- Novel disconnection patterns to valuable pharmacophores
- Practical and scalable chemistry
- Wide structural and functional group tolerance

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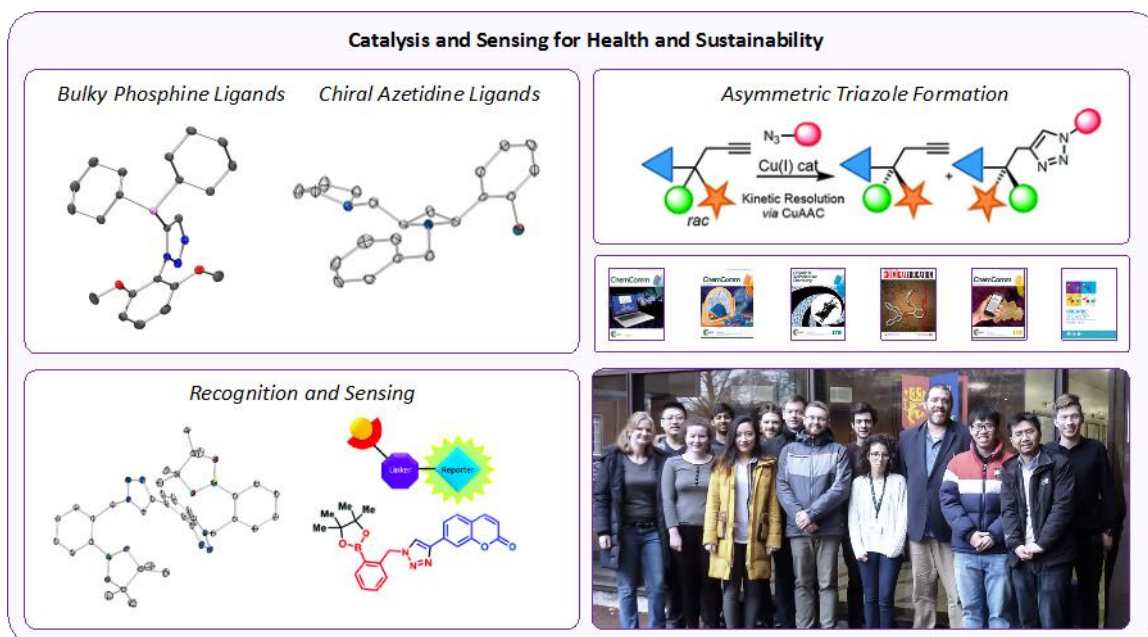
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PROF. JOHN S. FOSSEY
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Professor Fossey leads a team that conducts research on molecular synthesis with applications to catalysis, sensing and disease treatment. Collaboration, cooperation and community lies at the heart of the team's health and sustainability philosophy.

Recently the group's research on sensors for health has attracted funding from diabetes and cancer charities. Projects include collaborations with biological, medical and computational scientists. All projects are underpinned by molecular synthetic chemistry and a desire to create new molecules with well-understood and designed functionality.



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Twitter: @jsf_group

Rigid and concave, 2,4-cis-substituted azetidine derivatives: A platform for asymmetric catalysis. A. Yoshizawa, A. Feula, L. Male, A. G. Leach and J. S. Fossey, *Sci. Rep.*, **2018**, 8, 6541

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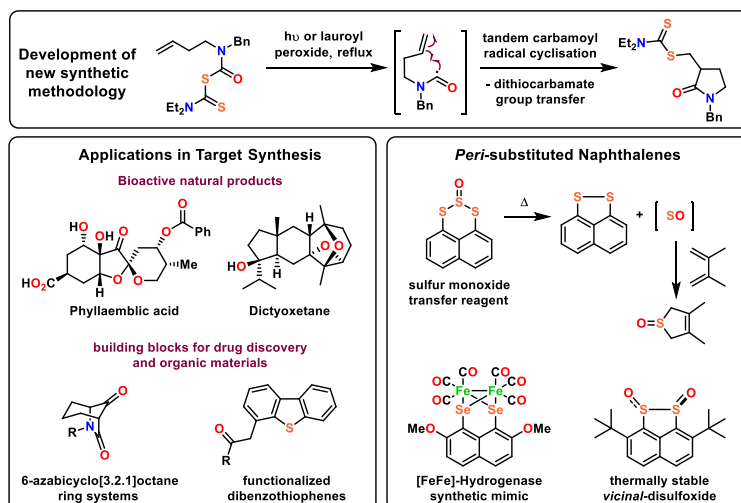
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DR. RICHARD GRAINGER

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Work in the group is centred on the development of new synthetic methods and strategies, and their application in the synthesis of organic molecules of biological or structural interest. Chemistry we are developing includes the use of reactive intermediates such as radicals and carbenes, photochemistry, cycloaddition reactions and organosulfur chemistry. We also have an active interest in the use of peri-substituted naphthalenes for the generation and stabilization of reactive functionalities.



Web: www.birmingham.ac.uk/staff/profiles/chemistry/granger-richard.aspx

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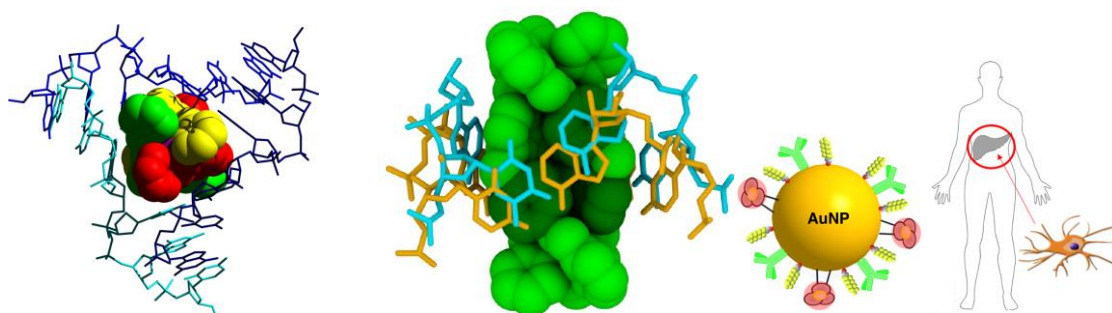
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PROF. MICHAEL HANNON

Email: m.j.hannon@bham.ac.uk

Bioinorganic Chemistry and Nanoscience: Anti-Cancer and Anti-viral Metallo-Drugs
Our research uses metal complexes in biology and medicine as both imaging agents and therapeutics. We develop synthetic chemistry (inorganic, organic, supramolecular) and apply biophysical methods to recognition of different DNA structures, and combine these with studies of activity, efficacy, and mechanism of action in living biological systems. In particular we work on the use of cylinder shaped metallo-drugs to non-covalently recognise DNA Y-shaped junctions (such as replication forks). We have started to expand the scope of this work into the field of nanotechnology through recognition and switching of DNA nanostructures. Other activities include metallo drug delivery and targeting and design of metallo imaging agents for a variety of imaging modalities and particularly for tracking administered therapeutic cells in the body.



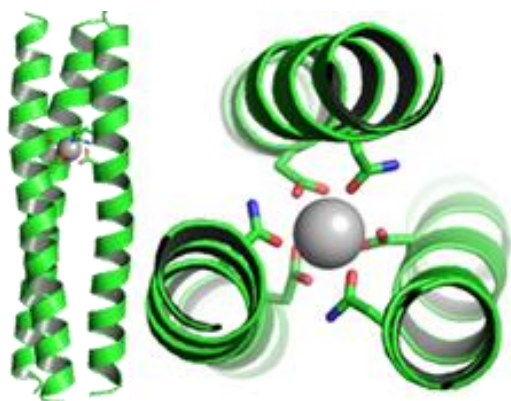
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Our research is focussed on the de novo (from “first-principles”) design of functional metalloproteins. Specifically we focus on the use of designed artificial miniature protein folds as novel ligands for metal ions. These miniature protein scaffolds offer unprecedented opportunities to exploit the advantages offered by biomolecules, yet with the simplicity more commonly encountered in small molecule inorganic chemistry complexes. Furthermore, we adopt the distinctive approach of using these as ligands for metal ions with no known biological role, but with attractive chemistries, in an effort to develop biology-chemistry hybrids with new functions for new applications. To date we have applied this concept to developing i) systems with which we can control sequence-selective DNA binding for potential gene regulation, as well as ii) generating novel MRI contrast agents for use in biomedical imaging.

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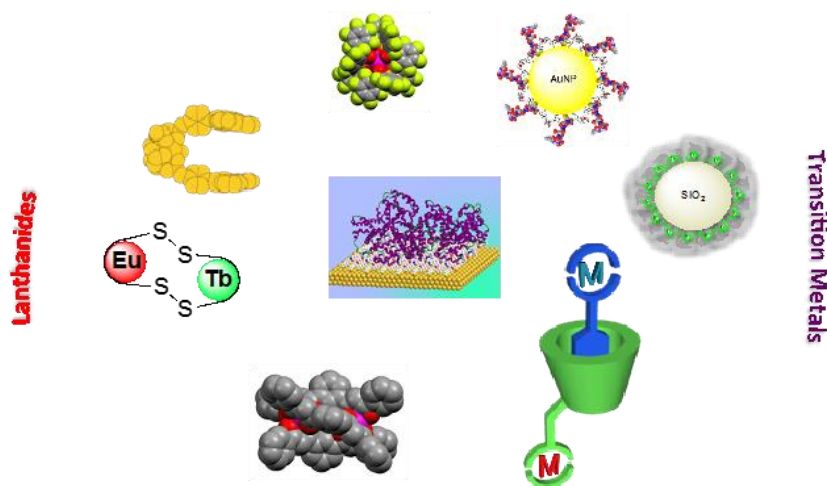
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Our research involves the design of luminescent molecular and nanosized towards the development of new materials for sensing, detection and energy conversion to tackle problems in improvement of healthcare for early diagnosis of disease, environmental detection or design of optoelectronic devices. Our projects involve synthetic and coordination chemistry, photophysics and nanoscience moving from supramolecular design and recognition to nanostructures with interdisciplinary teams of collaborators: medical scientists, dentists, biochemists, physicists and engineers. The projects involve lanthanide and transition metal complexes with recognition sites designs to target biomolecules such as DNA or "key" analytes in environmental pollution or biological function. In some projects we employ nanoparticles as scaffolds to carry metal complexes and targeting groups in cells for multimodal imaging. We study their targeted delivery in cells using peptide and other biomolecular recognition motifs. We use luminescence microscopy techniques based on the characteristic luminescence lifetime signal. To target the design of new materials and optoelectronic devices we study the modification of surfaces with metal complexes.

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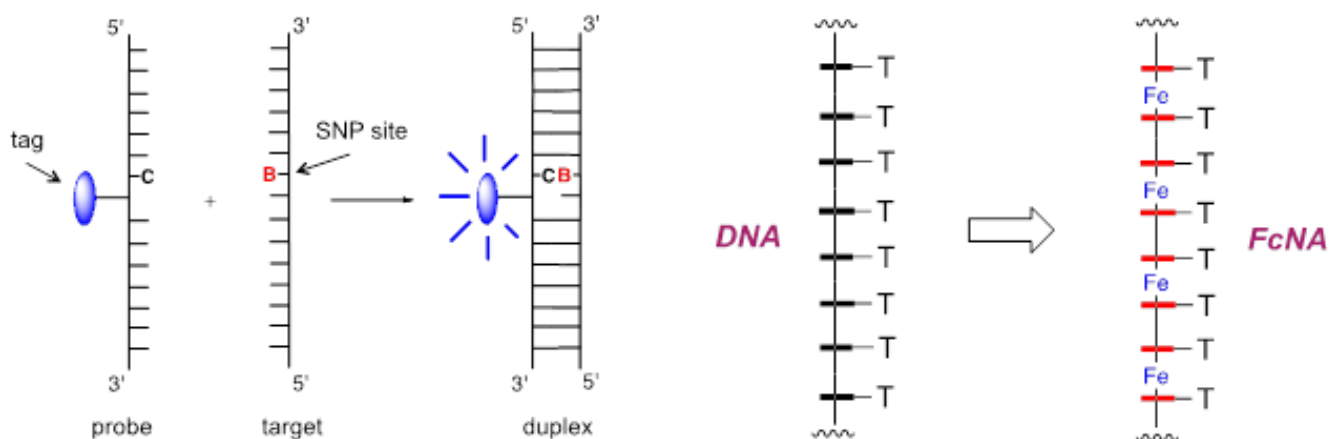
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The projects in our group fall within the areas of supramolecular and nucleic acid chemistry, typically involving small molecule organic/organometallic synthesis, which is then followed by DNA synthesis and then analysis using various spectroscopic or analytical techniques. One area of study involves the design of DNA probes that can detect changes at single nucleobase sites in sequences of DNA (SNP detection). The sensing of SNPs is important for our understanding of the origin of diseases that have a genetic component such as cancer and Alzheimer's. Other projects involve the synthesis of ferrocene compounds that show anticancer activity and their incorporation into nucleic acids to form artificial nucleic acids (e.g. ferrocene nucleic acid, FcNA) that show novel electrochemical and spectroscopic properties. Many of our projects involve collaborations with the medical researchers at Birmingham, for example in Cancer Sciences and Pharmacy.



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