IMAT APPLICATIONS 2024-25 ENTRY

Applications are now OPEN for the Inorganic Materials for Advanced Manufacturing (IMAT) doctoral programme.

Detailed information about this new DPhil course can be found on the Graduate Admissions section of the University's website (https://www.ox.ac.uk/admissions/graduate/courses) – search DPhil Inorganic Materials for Advanced Manufacturing). A summary of the course is given below.

About IMAT

The Inorganic Materials for Advanced Manufacturing (IMAT) training programme is a four-year doctoral course focusing on the design, synthesis and characterisation of new inorganic materials and features integrated academic/industrial courses. The course is jointly hosted by the Departments of Chemistry and Materials and has been designed in collaboration with 19 industrial partners, to provide a holistic understanding of all aspects of advanced materials manufacturing processes.

Students are trained initially (in the first six months) through a series of taught courses and a short industrial internship. From the second half of year one, you will focus primarily on your substantive research project.

Research projects:

The research projects for this programme will be allocated during the admissions process.
A list of the 36 projects available for the October 2024 entry is below. The list includes a summary of the project, some relevant background reading, and the contact details of the supervisors. Applicants are encouraged to read through the available projects and are required to list their three preferred projects (in order of preference) in their supporting statement. Further details on the research projects are available through direct contact with the supervisors or at the interview stage.

For any questions about the programme or the application, please contact the IMAT team at (imat-admin@chem.ox.ac.uk).

LIST OF PROJECTS AVAILABLE FOR 2024-25 ENTRY

Legend: Departments – (C) Chemistry, (E) Engineering, (M) Materials, (P) Physics

P1) Repurposing C-F bonds for nucleophilic fluoride delivery using metal hydride materials

Supervisors: Simon Aldridge (C), Véronique Gouverneur (C)

Summary: Methods for the formation of fluorine-containing molecules that avoid the intermediacy of HF are highly sought after. Repurposing existing F-containing 'waste' streams can by envisaged by developing metal-mediated processes for F abstraction and re- delivery. This project targets the direct conversion of metal hydrides to metal fluorides using F-containing waste, and the use of the derived M-F systems in nucleophilic fluoride delivery.

Relevant links: https://aldridge.web.ox.ac.uk
Enquiries: simon.aldridge@chem.ox.ac.uk, veronique.gouverneur@chem.ox.ac.uk

P2) Two-Dimensional Metal-Organic Frameworks

Supervisors: Harry Anderson (C), Martin Castell (M)

Summary: Two-dimensional metal-organic frameworks (2D MOFs) derived from transition metals and redox-active organic ligands behave as semiconductors, resulting in potential applications as chemiresistive sensors and electrocatalysts for fuel cells. This project will investigate the synthesis, structure and properties of new types of 2D MOFs using a combination of computer-aided molecular design, ligand synthesis, coordination chemistry and atomic-resolution scanning tunnelling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and charge-transport measurements.

Key publications: https://doi.org/10.1038/s41467-019-11009-y, https://doi.org/10.1039/c8cc02871k
Relevant links: http://hla.chem.ox.ac.uk/, https://users.ox.ac.uk/~mrc/
Enquiries: harry.anderson@chem.ox.ac.uk, martin.castell@materials.ox.ac.uk

P3) Engineering the Magnetism of New Solids

Supervisors: Simon Clarke (C), Stephen Blundell (P)

Summary: This project offers a special opportunity to join groups in two different Oxford departments (Chemistry and Physics) with common interests in functional materials and with complementary skills. New magnetic materials will be discovered, measured and controlled chemically with the aim of realising new crystal structures and controlling the magnetic interactions to introduce phenomena such as magnetic frustration and ferromagnetism.

Key publications: https://pubs.acs.org/doi/10.1021/acs.inorgchem.2c01773, https://pubs.acs.org/doi/10.1021/acs.inorgchem.0c02415, https://www.nature.com/articles/s41467-019-13450-5
Enquiries: simon.clarke@chem.ox.ac.uk

P4) Paramagnetic nanoparticle-DNA hybrids as programmable responsive contrast generators

Supervisors: Jason Davis (C), Jon Bath (P)

Summary: The generation of mesoporous nanoparticles with an interior that is both paramagnetically doped and potentially loaded with a therapeutic offers much to programmable theranostics. If one can sterically control the exposure of the interior particle void to the external solution than water and drug diffusion can be controlled. DNA is a programmable self-assembly material in which the strength and identity the of interactions between component parts can be designed using simple Watson-Crick base pairing rules. It can be used as a construction material for theranostic devices that can detect or release a drug and/or signal when a set of conditions are met. This project will design, fabricate and characterise these hybrid nanomaterials that can respond to biological cues associated with a disease state.

Key publications: J. Pellico, Chem. Comm. 2019 Vol. 55 Issue 59 Pages 8540-8543; C.M. Ellis, Chem Comm. 2023 Vol. 59 Issue 12 Pages 1605-1608; D. Yuan, Chem Comm. 2023 Vol. 59 Issue 40 Pages 6008-6011.
Relevant links: http://jjdgroup.co.uk, https://www.physics.ox.ac.uk/our-people/bath
Enquiries: Jason.davis@chem.ox.ac.uk

P5) MOF Molecular Films in Diagnostics

Supervisors: Jason Davis (C), Martin Castell (M)

Summary: Sufficiently conductive two-dimensional films have a capacitative fingerprint that is highly responsive to the dielectric changes associated with any molecular recognition event that occurs at their surface. Two-dimensional transition metal-organic frameworks (2D MOFs), including those that are redox responsive, have potential powerful applications in energy storage and diagnostics if they can be suitably receptor modified. This project will investigate the generation of electrochemically addressable transition metal MOF films, their capacitative charging, and the peripheral modification of these with biological receptors such that clinically-relevant biological targets can be detected.

Key publications: Baradoke et al, Anal Chem 2020, 92, 5, 3508-3511; Q. Xu et al, Analytical Chemistry 2015, 87, 1, 346-350; J. Piccoli et al, Analytical Chemistry 2018, 90, 5, 3005-3008; S. Kang et al, Anal Chem 2023, 95, 10, 4721-4727; Advanced Materials Interfaces 2023, 2202042.
Relevant links: http://jjdgroup.co.uk, https://users.ox.ac.uk/~mrc/
Enquiries: Jason.davis@chem.ox.ac.uk

P6) Designing nanocrystal synthesis at the atomic scale

Supervisors: Volker Deringer (C), Fernanda Duarte (C)
Collaborators: Robert Hoye (C)

Summary: Nanocrystals find application in diverse areas of chemistry and in energy materials, but their formation is an intricate process and only partly understood. We will develop new, machine-learning-driven approaches to understanding – and ultimately controlling – the formation of nanocrystals for optoelectronic and photovoltaic applications.

Key publications: *ACS* Nano **2021**, 15, 10775 (https://doi.org/10.1021/acsnano.0c08903), Nat. Rev. Mater. **2023**, *8,* 309 (https://doi.org/10.1038/s41578-023-00540-6).
Enquiries: volker.deringer@chem.ox.ac.uk

P7) Unlocking chemical complexity in machine learning for battery materials

Supervisors: Volker Deringer (C), Mauro Pasta (M)

Summary: Predicting new materials with large-scale computations and machine learning is a thriving research field. In this project, we will develop chemical ML models for structurally and compositionally complex inorganic materials – in particular, new glassy electrolytes for solid-state batteries – to be predicted and synthesised in the laboratory.

Key publications: *J. Phys. Energy* **2020**, 2*,* 041003 (https://doi.org/10.1088/2515-7655/abb011), *Nat. Rev. Mater.* **2023**, *8,* 309 (https://doi.org/10.1038/s41578-023-00540-6).
Enquiries: volker.deringer@chem.ox.ac.uk

P8) Understanding amorphous catalysts with machine-learning-driven simulations

Supervisors: Volker Deringer (C), Ludmilla Steier (C)
Collaborators: Michail Stamatakis (C), Robert Weatherup (M)

Summary: Amorphous materials find increasing use in catalysis, but their complex surface structures and their reactivity are far from fully understood. In this project, we will develop new machine-learning-driven approaches to predicting, and ultimately controlling, the structure of amorphous photocatalyst surfaces. We aim to understand the links between surface structure, composition, and product selectivity in the CO_2 reduction reaction, connecting simulations with state-of-the-art experimental characterisation.

Key publications: *J. Phys. Energy* **2022**, *4*, 042003 (https://doi.org/10.1088/2515-7655/ac7823), *Nat. Electron.* **2023**, *6*, 746 (https://doi.org/10.1038/s41928-023-01030-x).
Enquiries: volker.deringer@chem.ox.ac.uk

P9) Harnessing structural distortions in Prussian blue analogues for better Na-ion batteries

Supervisors: Andrew Goodwin (C), Mauro Pasta (M)

Summary: Prussian blue analogues (PBAs) are a diverse family of inorganic materials that show great promise as electrode materials in Na- and K-ion batteries — they have fast charge rates, high cyclability and can be made straightforwardly from inexpensive earth-abundant starting materials. We have recently uncovered a range of structural distortion mechanisms in K-ion PBAs that are of key importance to electrochemical performance, but the relevance of these to Na-ion PBAs is not yet known. This project will focus on combining detailed structural and electrochemical studies to a range of Na-ion PBAs to determine the nature and importance of distortion mechanisms in this family and with a view to developing new materials with improved electrochemical properties.

Key publications: Distortions in PBA cathodes (link, link)
Relevant links: Goodwin group (link), Pasta group (link)
Enquiries: andrew.goodwin@chem.ox.ac.uk

P10) Design of sustainable carbon-fibre 3D assemblies as catalysts and catalyst supports

Supervisors: Nicole Grobert (M), Kylie Vincent (C)

Summary: This project sits in the area of materials design for sustainable catalysis. The project will develop renewable, 3-dimensional carbon fibre assembly materials which will enable more efficient chemo-biocatalytic hydrogenation or electrochemical catalysis for generation of amine-containing chemicals via reduction of unsaturated bonds in nitrogen-containing molecules (eg nitro compounds, azides). It couples carbon materials design expertise from the Grobert group with innovative hydrogenation catalysis and electrocatalysis from the Vincent group.

Relevant links: http://www-grobert.materials.ox.ac.uk/, http://vincent.chem.ox.ac.uk/
Enquiries: nicole.grobert@materials.ox.ac.uk

P11) Topochemical modification of complex-oxide thin films

Supervisors: Michael Hayward (C), Susannah Speller (M)

Summary: Post-synthetic modification of transition-metal oxide thin films allows the synthesis of solid-state compounds that cannot be prepared by other routes. This allows the preparation of novel materials with properties such as superconductivity, magnetoresistance and spin-polarized conductivity.

Key publications: Topochemically reduced oxides
(https://pubs.acs.org/doi/10.1021/acs.inorgchem.9b00960), transition metal oxyhydrides
(https://onlinelibrary.wiley.com/doi/full/10.1002/anie.201800989,

https://www.nature.com/articles/s41467-017-01301-0), topochemical reduction of thin films (https://www.nature.com/articles/s41586-019-1496-5)
Enquiries: michael.hayward@chem.ox.ac.uk

P12) Scalable co-precipitation synthesis of transition metal oxide cathodes for sustainable sodium-ion batteries

Supervisors: Robert House (M), Paul Shearing (E)
Collaborators: The Faraday Institution, ISIS neutron source, Bill David (C/ISIS), Robert Weatherup (M), Peter Bruce (M)

Summary: Na-ion batteries are a cost-effective and more sustainable alternative to Li-ion batteries; however, the industrial synthesis of Na-ion cathode materials is currently performed via energy intensive solid-state shake-and-bake methods. This project will investigate the effects of shifting to co-precipitation synthesis to the structure, morphology, and electrochemical properties of Na-ion cathode materials, with the aim of facilitating an industry transition towards greener, more scalable manufacturing processes.

Key publications: https://www.nature.com/articles/s41586-019-1854-3, https://www.nature.com/articles/s41560-023-01211-0, https://theconversation.com/how-sodium-ion-batteries-could-make-electric-cars-cheaper-207342
Enquiries: robert.house@materials.ox.ac.uk

P13) Developing sustainable single crystals for ultrasensitive medical imaging devices

Supervisors: Robert Hoye (C), Simon Clarke (C)

Summary: High-quality medical imaging is critical for non-invasive diagnosis of, for example, malignant tumours, but is limited by the performance of the detectors currently available. We recently demonstrated BiOI single crystals to be 250 times more sensitive to X-rays than commercial a-Se detectors, opening up new opportunities to make medical imaging safer and faster. The key limiting factor is charge-carriers coupling to optical phonons, and in this project you will design and test new semiconducting materials in order to tune the structure, bond polarity and rigidity to further enhance performance and push the boundaries of ultra-sensitive radiation detectors.

Key publications: Bismuth oxyiodide (http://dx.doi.org/10.1038/s41563-022-01262-w), carrier-phonon interactions (http://dx.doi.org/ 10.1063/5.0071763), layered mixed-anion compounds (https://pubs.acs.org/doi/10.1021/ic8009964)
Relevant links: Hoye group: https://hoyegroup.web.ox.ac.uk/, Clarke group: https://clarkegroup.web.ox.ac.uk/home
Enquiries: robert.hoye@chem.ox.ac.uk

P14) Kesterite Indoor Photovoltaics for Sustainable Energy Harvesting

Supervisors: Robert Hoye (C), Peter Nellist (M)

Summary: The Internet of Things (IoT) is a central pillar of the fourth-industrial revolution, but the reliance on batteries as the energy supply for the hundreds of billions of smart devices presents a critical sustainability challenge. This project will develop kesterite indoor photovoltaics to more sustainably power IoT devices, particularly focussing on electron microscopy analyses of structural defects at interfaces and grain boundaries. The project also focuses on the integration of the photovoltaics developed with wearable electronics.

Key publications: Indoor photovoltaics (https://doi.org/10.1002/aenm.202002761), perspective on indoor photovoltaics (https://doi.org/10.1002/aenm.202100698)
Relevant links: Hoye group website: https://hoyegroup.web.ox.ac.uk/, Nellist Group website: https://www-stemgroup.materials.ox.ac.uk
Enquiries: robert.hoye@chem.ox.ac.uk

P15) Controlling Carrier Localisation in Mixed-Anion Perovskite-Inspired Materials

Supervisors: Robert Hoye (C), Robert Weatherup (Materials)
Collaborators: Aron Walsh (Imperial College London)

Summary: Lead-halide perovskites have revolutionised thin film photovoltaics, but are limited by their composition of toxic lead and limited stability. Working together with collaborators at Imperial College London, this project will take an interlinked experimental-computational approach to design, synthesise and develop the next generation of solar absorbers that can replicate the exceptional optoelectronic properties of lead-halide perovskites, but overcome their toxicity and stability limitations.

Key publications: Carrier localisation in NaBiS2: https://doi.org/10.1038/s41467-022-32669-3, Band-like transport in BiOI: https://doi.org/10.1038/s41467-023-38008-4 and https://doi.org/10.1021/acs.jpclett.3c01520
Relevant links: Hoye group website: https://hoyegroup.web.ox.ac.uk/, Weatherup Group website: https://emi.web.ox.ac.uk
Enquiries: robert.hoye@chem.ox.ac.uk

P16) Regulating transmembrane flux in paramagnetic nanomaterials for functional magnetic resonance imaging

Supervisors: Matthew Langton (C), Jason Davis (C)

Summary: This project will develop synthetic nanopores and transport systems for controlled ion and water transport across lipid bilayer membranes. Functional integration into paramagnetic nanoparticles and liposome to develop responsive MRI contrast agents will be explored.

Relevant links: https://www.chem.ox.ac.uk/people/matthew-langton#/
https://jjdgroup.co.uk
Enquiries: matthew.langton@chem.ox.ac.uk or jason.davis@chem.ox.ac.uk

P17) Photochromic main-group-lanthanide luminescent materials for sensing and information storage

Supervisors: Matthew Langton (C), Steve Faulkner (C)

Summary: This project will develop photochromic lanthanide systems incorporating main-group photoswitches, in which the emission can be modulated in response to different wavelengths of light. These will be applied to controlled anion sensing, and to access multi-state switchable luminescent materials for information storage.

Relevant links: http://faulkner.chem.ox.ac.uk https://langtonrg.web.ox.ac.uk
Enquiries: matthew.langton@chem.ox.ac.uk or Stephen.faulkner@chem.ox.ac.uk

P18) Photo-responsive and aggregation-induced emissive electrospun fluorescent fibres

Supervisors: Matthew Langton (C), Jin-Chong Tan (E)

Summary: This project will involve the chemical design and synthesis of inorganic molecular photoswitches with aggregation induced emission (AIE) properties, and interrogation of the photo-switching/photo-luminescence behaviour and guest binding capabilities (Langton group). These systems will be fabricated into stimuli-responsive photoluminescent electrospun fibres (Tan group), for applications in sensing and guest binding and delivery.

Relevant links: http://faulkner.chem.ox.ac.uk https://eng.ox.ac.uk/mmclab/
Enquiries: matthew.langton@chem.ox.ac.uk

P19) Electrospinning solid oxide electrolysis cells – hydrogen production for the energy transition

Supervisors: Katharina Marquardt (M), Nicole Grobert (M)
Collaborator: Mark Wilson (C)

Summary: Sol-gel Electrospinning of ceramic fibers offers the possibility to manufacture ceramics with tuneable macroscopic shape, volume, density, and porosity (Grobert) enabling advanced SOEC design. Different choices of surfactants further open the possibility of designing the crystal facets with the best catalytic and stability properties as well as designing the texture and interface population in densified ceramics. Such choices will be informed by modeling (Wilson). This is a unique possibility to enable the synthesis of preferential interface populations (Marquardt) in SOEC for enhanced hydrogen production.

Relevant links: Marquardt (link), Grobert group (link), Wilson group (link)
Enquiries: Katharina.marquardt@materials.ox.ac.uk and Nicole.grobert@materials.ox.ac.uk

P20) **Leveraging Bismuth Redox Catalysis to Build Difficult Bonds**

Supervisors: Meera Mehta (C), Simon Aldridge (C)
Collaborator: Christiane Timmel (C)

Summary: Up to 90% of chemical products require a catalytic step somewhere in their preparation. The catalysts that the manufacturing sector relies on to enable these transformations are often based on precious and depleting transition metals. Here, a new family of sustainable redox-active bismuth catalysts are targeted. These catalysts will be applied in halogen atom transfer processes (XAT) to build otherwise difficult C–C and C–N bonds that are of great importance to pharmaceutical and materials science. This project involves skills in organic and inorganic synthesis, spectroscopy, and computation chemistry.

Key publications: Pnictogen catalysis (*Angew. Chem. Int. Ed.* 2020, 59, 2715), radical chemistry (*Nature Chem.* 2014, 6, 315)
Relevant links: mehtalab.co.uk, aldridge.web.ox.ac.uk
Enquiries: meera.mehta@chem.ox.ac.uk, simon.aldridge@chem.ox.ac.uk

P21) **Clusters as Shapeshift Ligands for Sustainable Cooperative Catalysis**

Supervisors: Meera Mehta (C), Michael Neidig (C)
Collaborator: John McGrady (C)

Summary: A new class of intramolecular cooperative catalysts that feature sustainable d-block and group 13 elements mounted on a Zintl cluster will be prepared. This family of catalysts will then be employed to mediate two categories of transformations of high value to the manufacturing sector: 1) olefin functionalisation reactions; 2) hydroformylation reactions. This project involves skills in organic and inorganic synthesis, spectroscopy, and computational chemistry.

Key publications: Cluster chemistry (*J. Am. Chem. Soc.* **2022**, 144, 46, 21213–21223), 3d metal catalysis (*J. Am. Chem. Soc.* **2018**, 140, 11872–11883)
Relevant links: mehtalab.co.uk, https://theneidiglab.web.ox.ac.uk/home
Enquiries: meera.mehta@chem.ox.ac.uk, michael.neidig@chem.ox.ac.uk

P22) **Organometallic Iron Cluster Catalysts for Sustainable Chemical Synthesis**

Supervisors: Michael Neidig (C), John McGrady (C)

Summary: Organometallic iron clusters have been identified as active catalytic species in iron-catalysed cross-couplings, representing a new paradigm in organoiron catalysis. Furthermore, iron clusters have been implicated as a broader class of sustainable catalysts for transformations across the breadth of modern chemical synthesis (including olefin functionalisations). This project seeks to revolutionise organoiron catalysis by expanding the utility of this exciting new class of cluster catalysts across a variety of carbon-carbon and carbon-heteroatom bond forming reactions, combining inorganic synthesis, spectroscopy,

computational chemistry and reactivity studies to define the unique electronic structure and bonding properties underlying their reactivities.

Key publications: https://pubs.acs.org/doi/10.1021/jacs.6b03760
https://pubs.rsc.org/en/content/articlelanding/2018/sc/c8sc02915f
Enquiries: michael.neidig@chem.ox.ac.uk

P23) High fluoride mobility layered double hydroxide electrolytes

Supervisors: Dermot O'Hare (C), Mauro Pasta (M)

Summary: In the future batteries with energy densities above 800 Whkg^{-1} will be required. Several "post lithium-ion" battery technologies – such as fluoride-ion batteries (FIBs) – are being explored to address this need. This project will investigate the synthesis of new fluoride containing layered double hydroxide nanosheets liquid dispersions/gels in order to create stable and safe high F$^-$ mobility electrolytes: this project will integrate the chemical design/synthesis of novel layered double hydroxide (O'Hare group) and the electrochemical characterisation of electrolytes and battery systems (Pasta group) to produce new high-performance FIBs.

Relevant links: O'Hare group (link); Pasta group (link)
Enquiries: dermot.ohare@chem.ox.ac.uk, mauro.pasta@materials.ox.ac.uk

P24) Plasma-assisted olefin depolymerisation

Supervisors: Dermot O'Hare (C), Grant Ritchie (C)

Summary: Plasma-assisted catalysis provides a way of 'gaming' the thermodynamic landscape, making new chemical pathways available and/or lowering barriers to existing pathways, without the required increase in temperature. This project seeks to elucidate key parameters in the important plasma regions - sensitive end-point chemistry, active gas-phase species and surface and gas phase properties - with a view to optimising catalyst materials and reactor design for the depolymerisation of olefins into hydrocarbons, hydrogen and other nitrogen-containing small molecules by atmospheric nitrogen plasma.

Relevant links: O'Hare group (link); Ritchie group (link)
Enquiries: dermot.ohare@chem.ox.ac.uk, grant.ritchie@chem.ox.ac.uk

P25) From biomass to high-value chemicals: synergistic experimental-computational studies of biomass-derived glycerol to acrolein over dilute alloy catalysts

Supervisors: Michail Stamatakis (C), Edman Tsang (C)

Summary: Acrolein is the simplest unsaturated aldehyde and a key molecule in the industrial manufacture of acrylic acid and polymers, but its production is based on fossil feedstocks (propylene) and is therefore subject to sustainability concerns. While glycerol, derived as a

by-product of biomass-to-biofuels conversion, can serve as a "green feedstock" for acrolein production, selectivity challenges are encountered in the pertinent dehydration processes, while the formation of coke precursors via acrolein or glycerol oligomerisation leads to risks of catalyst deactivation. This project adopts computational catalyst screening methods to identify promising dilute alloy catalysts composed of transition metals doped into Cu hosts for the conversion of glycerol to acrolein, and will inform experimental catalyst discovery efforts.

Relevant links: http://stamatakislab.org/ ; https://tsang.web.ox.ac.uk/
Enquiries: michail.stamatakis@chem.ox.ac.uk

P26) Nitro reduction at carbon for manufacture of amine-containing chemicals: a combined computational and experimental study of mechanisms and selectivity

Supervisors: Michail Stamatakis (C), Kylie Vincent (C)

Summary: Amine-groups are widespread in pharmaceuticals, agrochemicals and many other important chemicals. An important route to their synthesis is via reduction of nitro groups, but available nitro reduction methods suffer from limited selectivity, rare-metal catalysts or use of heavy metals. This project builds on demonstrations of nitro group reductions at carbon, either via electrocatalysis or hydrogenation catalysis, and uses a combination of experimental methods (electrochemistry, GC, NMR, IR spectroelectrochemistry) to feed into a computational study of mechanism (via density functional theory and kinetic Monte Carlo) aiming at elucidating means of tuning selectivity to the amine product.

Relevant links: http://stamatakislab.org/ ; http://vincent.chem.ox.ac.uk/
Enquiries: kylie.vincent@chem.ox.ac.uk

P27) CO_2 Reduction over Perovskite Materials: elucidating reaction selectivity via computational modelling and operando experiments

Supervisors: Michail Stamatakis (C), Robert Weatherup (M)
Collaborators: Ludmilla Steier (C)

Summary: Breakthroughs in the electrochemical conversion of CO_2 to $C_XH_YO_Z$ are urgently needed in our race to replace fossil feedstocks with renewable ones for the production of sustainable fuels and chemicals; in this context, copper stands out as a promising electrocatalyst which can generate more than 16 products, yet so far with only poor selectivity. Crucially, however, several reports suggest that the presence of Cu^+ and Cu^{2+} yields higher selectivity towards multi-carbon products such as ethylene, and thus, this project aims to explore La_2CuO_4 and related perovskite oxides to understand the underlying mechanisms and the effect of the oxidation state of Cu on selectivity. The project adopts first principles-based computational chemistry approaches in tandem with operando experiments to elucidate the active site of the perovskite under reaction conditions, and explore approaches such as Ba doping to stabilise the Cu in a desired state and prevent nanoparticle exsolution.

Key publications: (doi: 10.1088/2515-7655/ac7823); (doi: 10.1063/5.0083251); (doi: 10.1039/C5CP04058B)
Relevant links: http://stamatakislab.org/; https://emi.web.ox.ac.uk/; https://www.chem.ox.ac.uk/people/ludmilla-steier
Enquiries: michail.stamatakis@chem.ox.ac.uk , robert.weatherup@materials.ox.ac.uk

P28) Towards the discovery of novel photocatalysts for the conversion of carbon dioxide to green chemicals

Supervisors: Ludmilla Steier (C), Simon Clarke (C)

Summary: This project will be at the forefront of exploring new catalysts for the photocatalytic conversion of CO_2 to green chemicals. In particular, layered oxide chalcogenide and perovskite chalcogenide compounds with strong light absorption in the visible region of the solar spectrum will be targeted using solid-state synthesis (Clarke group) and studied in photocatalytic reactions (Steier group) with a focus on building an understanding of the chemical structure and catalytic properties including energy conversion efficiency, product selectivity and catalyst activity over time. You will be exposed to a wide range of techniques for bulk and thin-film synthesis, structural characterisation, spectroscopy and catalytic characterisation and hence develop a thorough understanding of how to tune structural, chemical and optical properties to enhance photocatalysis.

Key publications: oxychalcogenides: https://pubs.acs.org/doi/10.1021/ic8009964 and https://pubs.acs.org/doi/10.1021/ja8063414
perovskite sulfides: https://doi.org/10.1021/acs.chemmater.8b04178
perovskites in catalysis: https://www.science.org/doi/10.1126/science.aam7092
particulate photocatalysts: https://www.nature.com/articles/natrevmats201750
defects in photocatalysts: https://www.nature.com/articles/s41563-020-00868-2
Enquiries: ludmilla.steier@chem.ox.ac.uk; simon.clarke@chem.ox.ac.uk

P29) Atomic scale catalyst design driven by operando atmospheric-pressure XPS

Supervisors: Ludmilla Steier (C), Robert Weatherup (M)
Collaborators: Volker Deringer (C), Michail Stamatakis (C)

Summary: The study of catalyst surfaces under realistic or close to realistic reaction conditions is vital for the understanding and design of new catalysts. Material properties such as oxidation states and the Fermi level/work function are highly sensitive to the environment and can vary significantly when measured under ultra-high vacuum conditions. With the recent development of monolayer graphene membranes, atmospheric pressure X-ray photoelectron spectroscopy (AtmPXPS) can measure material properties at pressures in excess of 1 bar, allowing access to the conditions of industrial catalysis. In this project, the student will manufacture novel particulate and thin film photocatalysts using atomic layer deposition (ALD) directly coupled to the AtmPXPS setup which will allow the study of their nucleation and growth mechanism before focusing on the evolution of their surface

properties under photocatalytic reaction conditions. This will shed light on the catalytically active sites during the hydrogenation of CO_2 or the splitting of water into green hydrogen.

Key publications: https://pubs.acs.org/doi/10.1021/acs.jpclett.6b00640
https://link.springer.com/article/10.1007/s11244-018-1075-2
https://pubs.acs.org/doi/abs/10.1021/acsnano.5b03694
Enquiries: ludmilla.steier@chem.ox.ac.uk; robert.weatherup@materials.ox.ac.uk

P30) Synthesis of Inorganic Molecular Compasses

Supervisors: Christianne Timmel (C), Harry Anderson (C)

Summary: This project will focus on the design, synthesis and characterisation of inorganic molecular compasses. The optical properties of such "compasses", during light- induced electron transfer reactions, can be surprisingly sensitive to magnetic fields. Starting with a BODIPY-Al^{3+}-porphyrin-C_{60} triad, we will optimise the molecular structure for maximum magnetic sensitivity using techniques such as EPR and picosecond transient absorption spectroscopy.

Key publications: https://doi.org/10.1038/s41467-019-11655-2
https://doi.org/10.1007/s00723-021-01379-2
Relevant links: http://hla.chem.ox.ac.uk/, http://timmel.chem.ox.ac.uk
Enquiries: christiane.timmel@chem.ox.ac.uk, harry.anderson@chem.ox.ac.uk

P31) Catalytic CO_2 Hydrogenation over Single atom/cluster on Supports

Supervisors: Edman Tsang (C), John McGrady (C)
Collaborators: James Kwan (E), Michail Stamatakis (C)

Summary: This project is concerned with novel synthesis, testing, and characterization of single transition metal atoms and small clusters on zeolite and related inorganic supports as new inorganic catalytic materials for a wide range of CO_2 hydrogenation to useful alcohols/hydrocarbons. Rational synthesis using various physiochemical synthetic techniques to establish the structures for optimal performance will be combined with advanced material characterization including diffraction, electron microscopy, and computation to guide the synthesis and materials tested for the reaction.

Key publications: https://www.nature.com/articles/s41467-023-36339-w
https://pubs.acs.org/doi/abs/10.1021/jacs.1c01097]
Enquiries: edman.tsang@chem.ox.ac.uk

P32) Electrocatalytic CO$_2$ Reduction to Hydrocarbons over Modified Cu Catalysts

Supervisors: Edman Tsang (C), Dermot O'Hare (C)

Summary: Electrocatalytic CO$_2$ reduction in aqueous medium requires a proper balance of protons, hydroxyls, carbonate ions and alkali-metal ions at the cathode and anode. By using Cu based catalysts, we have recently reported a pure-water-fed membrane–electrode–assembly system for CO$_2$ reduction to ethylene by integrating an anion-exchange membrane and a proton-exchange membrane, respectively, under forward bias with excellent stability at high Faradaic efficiency and current density towards ethylene. Here we propose to systematically investigate the support effects for the Cu phase to optimise best catalytic selectivity, activity and lifetime under neutral pH and gain controls in catalytic performance.

Key publications: https://www.nature.com/articles/s41560-023-01415-4;
https://www.cell.com/chem/pdf/S2451-9294(20)30540-4.pdf
Enquiries: edman.tsang@chem.ox.ac.uk; dermot.ohare@chem.ox.ac.uk

P33) Simplifying operation of cytochrome P450 monooxygenases for fine chemical manufacturing

Supervisors: Kylie Vincent (C), Luet Wong (C)
Collaborators: Stephen Bell (Univ of Adelaide, AUS); Sarah Barry (Kings College London)

Summary: Biocatalysis is increasingly important in the manufacture of fine chemicals, including pharmaceuticals, aromas and flavours. This project focuses on cytochrome P450 monooxygenase enzymes which catalyse a vast array of oxygen-atom insertions. The project sets out to develop smarter routes to delivery of reducing equivalents to these enzymes based on interfacing hydrogenase with carefully selected carbon-based supports.

Relevant links: https://www.chem.ox.ac.uk/people/kylie-vincent
https://www.chem.ox.ac.uk/people/luet-wong
Enquiries: kylie.vincent@chem.ox.ac.uk

P34) Next Generation Batteries: Precision Polymers Integrated with Advanced Inorganic Materials For High Performance, Recyclable Solid State Batteries

Supervisors: Charlotte Williams (C), Georgina Gregory (C)
Collaborators: Peter Bruce (M)

Summary: Achieving net-zero carbon emissions requires better batteries; here polymer binders and electrolytes for solid state batteries are targeted to show high conductivity, mechano-chemical properties, electrochemical stability and to facilitate large-scale cell manufacturing. The project applies high selectivity and control polymerization catalysts to produce block and copolymers from oxygenated monomers and explores structure-performance relationships in next generation lithium and sodium ion batteries.

Key publications: https://doi.org/10.1021/jacs.2c06138
Relevant links: Home - Charlotte Williams Research (ox.ac.uk)
Enquiries: charlotte.williams@chem.ox.ac.uk

P35) **Using Carbon Dioxide to Make High Performance, Recyclable Engineering Polymers: Combined Experimental and Machine Learning Investigations**

Supervisors: Charlotte Williams (C), Clive Siviour (E)
Collaborators: David Clifton (E), Georgina Gregory (C)

Summary: New catalysts and polymers using carbon dioxide and bio-derived heterocycles (e.g. epoxides, lactones, cyclic carbonates, anhydrides) are developed to produce engineering thermoplastics. These polymers are targeted for uses in electronics and automotive sectors, so understanding structure-performance-recycling behaviours is critical; experimental work is underpinned by machine learning to predict polymer properties using PolyAGM, an in-house database and software tool.

Key publications: https://doi.org/10.1021/jacs.9b13106; https://doi.org/10.1021/jacs.2c06921
Relevant links: Home - Charlotte Williams Research (ox.ac.uk)
Enquiries: charlotte.williams@chem.ox.ac.uk

P36) **Systematic Modelling of Disorder B/C/N Composites**

Supervisors: Mark Wilson (C), Nicole Grobert (M)
Collaborators: Volker Deringer (C)

Summary: B/N/C composites can possess potential significant electronic and thermoelectric properties in the bulk, as thin films, nanotubes or spun fibres. Effective modelling is complex owing to the subtle balance of interactions resultant from small differences in electronegativities. We will develop (relatively simple) potential models which with allow greater insight into these key properties.

Relevant links: Wilson group (https://www.chem.ox.ac.uk/people/mark-wilson),
Grobert group (https://www.materials.ox.ac.uk/peoplepages/grobert.html)
Enquiries: mark.wilson@chem.ox.ac.uk

P37) **Probing Polymer-inorganic Interfaces using Nanoindentation: Implications for Advanced Material Design**

Supervisors: Georgina Gregory (C), David Armstrong (M)

Summary: Synthesizing polymers that interface effectively with inorganic substrates is pertinent to various industrial applications, such as enhanced durability, chemical resistance, and controlled conductivity. This project will explore the interfacial chemistry between polymers and inorganic substrates, utilizing nanoindentation as a primary investigative tool. It involves the synthesis of well-defined polymers using controlled polymerization strategies

such as metal-catalysed ring-opening polymerization and ring-opening copolymerization. Polymer end-groups and side chains will be chemically modified to systematically investigate and correlate the mechanical properties at the nano-scale, as revealed by indentation techniques, with the underlying chemical interactions. The objective is to establish insights essential for the design of advanced composite materials with tailor-made functionalities.

Relevant links: https://www.chem.ox.ac.uk/people/georgina-gregory
Enquiries: georgina.gregory@chem.ox.ac.uk

P38) Manufacturing to tune the grain boundary network in fusion shielding materials

Supervisors: Katharina Marquardt (M), David Armstrong (M)

Summary: Manufacturing of next generation nuclear shielding materials is critical to enable sustainable large scale low carbon-footprint energy coverage. Yet different manufacturing routes result in materials with different properties and often these variations are related to changes in microstructure. We will evaluate the effect of different low activation binder phases on the manufacturability and related property variations to the study of grain and phase boundary networks.

Relevant links: Marquardt group, Armstrong group
Enquiries: Katharina.marquardt@materials.ox.ac.uk

P39) Next generation solid state battery electrolytes: determining how the polycrystalline ceramic electrolyte microstructure and grain boundaries control performance

Supervisors: Katharina Marquardt (M), Peter Bruce (M)
Collaborator: Dominic Melvin (M)

Summary: Solid-state batteries (SSB) with ceramic electrolytes are critical to move our society away from high-carbon footprint energy production, enabling storage and transport of energy. While it is known that grain boundaries affect the performance of the solid-state ceramic electrolytes – how they do so is not known. This project is focused on characterizing the ceramic electrolytes GB-crystallography, GB-network, and GB-evolution using advanced electron microscopy. Synchronized electrochemical measurements will link electrical properties to the GB-structure and -network. Initially we focus on cubic $Li_7La_3Zr_2O_{12}$ (LLZOs), one of the most favourable electrolyte ceramics, later extending to the sulphides such as Li_6PS_5Cl.

Relevant links: Marquardt group, Bruce group.
Enquiries: Katharina.marquardt@materials.ox.ac.uk, peter.bruce@materials.ox.ac.uk

P40) **Bridging Structure and Performance at the nanoscale for Advanced mRNA Vaccine Delivery**

Supervisors: Molly Stevens (E), Professor Peter Nellist (M)

Summary: Nanocarriers have revolutionized medicine, notably expediting anti-COVID-19 vaccine development. Yet the major obstacle in their clinical application is the challenging control of nanoscale particle synthesis, leading to heterogeneity and impeding manufacturing and regulatory processes. This project aims to enhance organic and inorganic nanoformulations for mRNA vaccine delivery by leveraging the unparalleled insights into the structure-function-performance relationship, enabled by the combination of SPARTA® analysis (Molly Stevens' group) and high-resolution electron imaging (Peter Nellist's group).

Relevant links: Stevens Group, Peter Nellist's group
Enquiries: molly.stevens@dpag.ox.ac.uk, m.stevens@imperial.ac.uk, peter.nellist@materials.ox.ac.uk

P41) **Nanozyme-enhanced diagnostics: leveraging structural insights for performance optimisation**

Supervisors: Molly Stevens (E), Paul Bagot (M)

Summary: The COVID-19 pandemic has familiarised us all with the significance of point-of-care diagnostic tools for rapid, reliable, and accessible testing. Nanozymes (Molly Stevens' group), with their exceptional catalytic properties and stability, hold the promise of unmatched sensitivity for point-of-care diagnostic biosensors. Atom Probe Tomography (Paul Bagot's group) enables the structural and chemical characterisation of nanozymes with an unprecedented level of detail. The gained new insights into structure-function relationship will be leveraged to optimise the new generation of nanozymes for enhanced CRISPR-based diagnostics.

Relevant links: Stevens Group, R.A.P.T.O.R.
Enquiries: molly.stevens@dpag.ox.ac.uk, m.stevens@imperial.ac.uk, paul.bagot@materials.ox.ac.uk