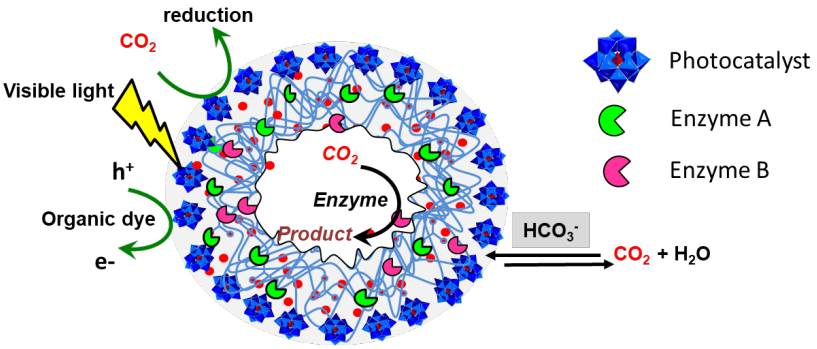
Construction of multi-catalytic protocells for effective CO_2 fixation and conversion

About the project or challenge area: The rapid growth of carbon dioxide (CO_2) in the environment due to anthropogenic activity has resulted in increasing global warming and climate change. Hence, there is a constant quest to develop new methods and technologies to reduce the levels of CO_2. Significantly, plants and a few bacteria utilize CO_2 in photosynthesis and produce glucose as a source of energy. However, the natural CO_2 fixation is too slow as a process to fix all the environmental CO_2. One new area where colloidal-scale structures could make a significant breakthrough is in the formation of artificial-cell-like materials (protocells). Much of the inspiration for this approach comes from mimicking key aspects of the living cells, albeit with a large degree of simplification. This project aims to utilize functional biotic (enzymes) and abiotic (catalytic inorganic nanoparticles) components for the construction of programmable protocell architectures (multi-catalytic reactors***, see the schematic below***) and handlable devices for applications in CO_2 fixation and environmental remediation. Overall, design and construction of new affordable materials with small-scale structures and biomimetic properties is expected to be of great importance in wide-ranging applications such as sensing, storage and release, and controlled catalysis.

Why choose this opportunity? The focus of your project will be on synthesis of functional inorganic nanoparticles, bio/photocatalysis and microfabrication technologies which will provide an excellent platform to learn about the design of functional materials at various length scales and their practical applications. Your work in this area can make a real impact on global challenges, such as multi-catalytic compartmentalized colloidal-scale objects for energy storage, carbon fixation, water splitting, health and personal care and advanced composite micro-engineering. You will develop and increase your expertise in broad chemical synthesis and characterization techniques, whilst becoming familiar with the fundamentals of nanomaterials, self-assembly and bio-/photocatalysis. Furthermore, this project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. You will also develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.



Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: Ideally you will already have skills and knowledge in general preparative chemistry, teamwork and time management.

Bench fees: A bench fee of £7000 is required.

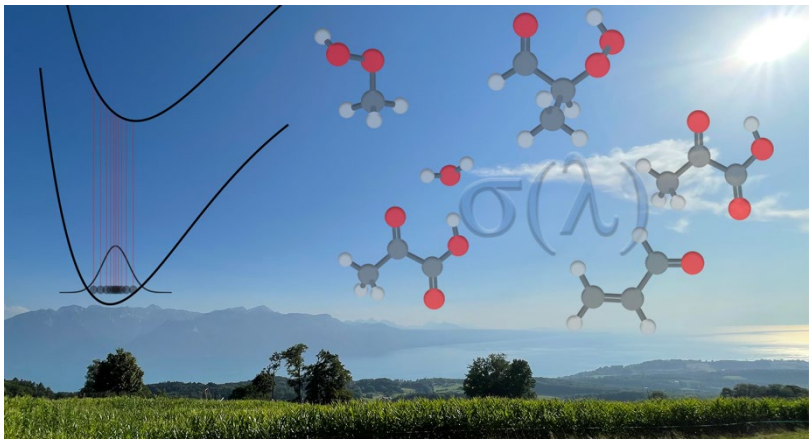
How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be **Dr Avinash Patil**, in the School of Chemistry. You can contact him at +44 (0) 117 3317215 or email avinash.patil@bristol.ac.uk

Find out more about your prospective research program: This paper explains the design and construction of catalytic protocells. https://www.nature.com/articles/s41467-019-13759-1

Calculating photoabsorption cross-sections for atmospheric volatile organic compounds

About the project or challenge area: Understanding the chemical and photochemical reactions taking place in the atmosphere is paramount to predicting its composition. A large number of the atmospheric volatile organic compounds (VOCs) are transient species, presenting a real challenge for experimentalists to characterise them. Computational chemistry is often used to provide missing experimental data to the models used to simulate the atmosphere composition. While ground state properties of molecules are rather simple to compute, obtaining information about their excited electronic states constitutes a real challenge. Key analysis of experimental data would nevertheless require properties of molecules such as absorption spectra (or photoabsorption cross-sections), or information about the reactivity of a VOC following light absorption. In this project, you will learn how to use advanced computational techniques aiming at calculating photoabsorption cross-sections and simulating the excited-state dynamics of a molecule.



Why choose this opportunity? The focus of your project will be on theoretical and computational chemistry, which will provide an excellent platform to learn about the properties of molecules. Your work in this area can make a real impact on global challenges, such as the influence of photochemical reactions for the removal of transient VOCs in the atmosphere and their contribution to the formation of secondary pollutants. You will develop and increase your expertise in computational chemistry and using quantum-chemical packages, whilst becoming familiar with the fundamentals of the interaction between light and molecules. Furthermore, this project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. You will also develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: Ideally you will already have skills and knowledge in basic computational chemistry and the use of Linux, teamwork and time management.

Bench fees: A bench fee of £3000 is required.

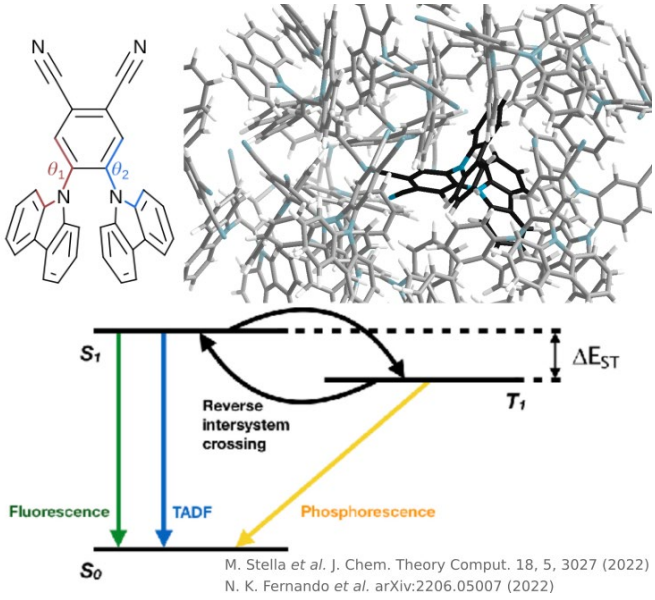
How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Basile Curchod, Associate Professor in the School of Chemistry. You can contact him by email basile.curchod@bristol.ac.uk.

Find out more about your prospective research program: This recent work from our group provides some general background on calculating photoabsorption cross-section for atmospheric molecules:

Calculating Photoabsorption Cross-Sections for Atmospheric Volatile Organic Compounds
ACS Earth Space Chem., 2022, 6, 207–217 https://pubs.acs.org/doi/10.1021/acsearthspacechem.1c00355

Simulating Next Generation Organic Light Emitting Diodes



About the project or challenge area: Organic semiconductors have a number of advantages for use in devices such as light emitting diodes (LEDs), including light weight, low cost and flexibility. However, the current generation of organic LEDs (OLEDs) are based on molecules containing scarce and expensive heavy metals such as Ir and Pt, motivating the development of OLEDs based on molecules exhibiting thermally activated delayed fluorescence (TADF). TADF-based emitters can be purely organic, avoiding the need for heavy metals and leading to efficient and environmentally-friendly devices. Given the vast number of potential TADF emitters, computational chemistry has an important role to play in identifying new TADF molecules, for example by calculating key properties which govern TADF, such as the singlet-triplet splitting. However, this is complicated by the need to account for factors such as disorder and environmental effects, which can have a strong influence on properties. This project will use density functional theory to simulate TADF-based emitters, with the aim of providing new insights into their electronic structure.

Why choose this opportunity? The focus of your project will be on using computational chemistry to simulate TADF-based OLEDs, which will provide an excellent platform to learn about the use of computational chemistry for practical applications. Your work in this area can make a real impact on global challenges, such as the development of emitters for environmentally friendly OLEDs. You will develop and increase your expertise in computational chemistry and coding, whilst becoming familiar with the fundamentals of electronic structure. Furthermore, this project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. You will also develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: Ideally you will already have skills and knowledge required to understand concepts related to electronic structure, as well as an enthusiasm for computational research and coding, and teamwork and time management.

Bench fees: A bench fee of £2500 is required.

How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Laura Ratcliff, Research Fellow in the School of Chemistry. You can contact her at laura.ratcliff@bristol.ac.uk

Find out more about your prospective research program: *High-efficiency organic light-emitting diodes from delayed fluorescence,* Nature **492**, 234 (2012), https://www.nature.com/articles/nature11687

New photocatalytic strategies for organic synthesis with ketyl radicals

About the project or challenge area: Visible-light photoredox catalysis is becoming an increasingly valuable tool in organic synthesis. This is because it allows versatile free radical intermediates to be formed by single electron transfer (SET) reactions under mild conditions by simply irradiating reaction mixtures with common household lightbulbs or LEDs. However, for particularly challenging SET reactions, photoredox catalysis fails, and therefore stoichiometric amounts of strong oxidants or reductant are required instead. This is often the case for ketyl radicals, which are highly useful synthetic intermediates that can be accessed by single electron reduction of carbonyls, such as aldehydes or ketones. Typically, this challenging reduction requires the use of super-stoichiometric strong metal reductants, which leads to a lot of waste and limits the sustainability of these reactions.

In this project, you will investigate new strategies that allow ketyl radicals to be generated under mild catalytic conditions and without the use of stoichiometric reductants. This will be achieved by designing redox-active derivatives of aldehydes and ketones that can be transformed into ketyl radicals using photoredox catalysis (Figure 1). These new reagents will enable us to significantly expand the scope of ketyl radical chemistry beyond what is currently possible with stoichiometric reductants.

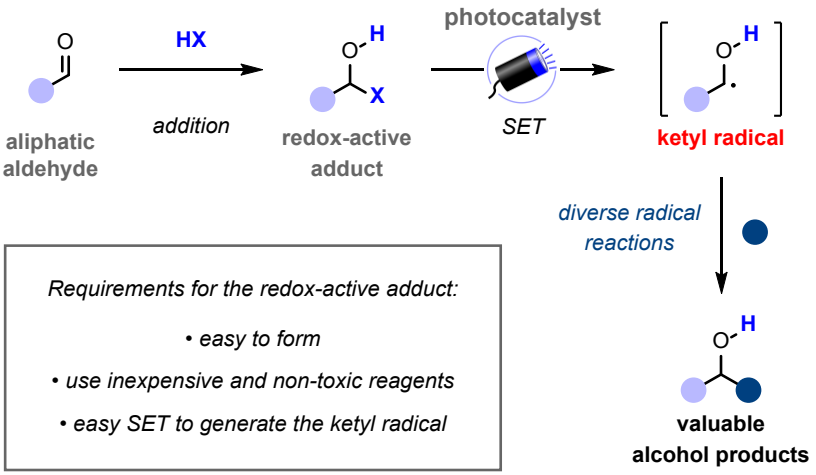


Figure 1

Why choose this opportunity? The focus of your project will be to develop new approaches to ketyl radicals using visible-light photoredox catalysis, which will provide an excellent platform to learn about photochemistry, radical chemistry, and the development of new synthetic methodologies. Your work in this area will provide new, sustainable reactions that can be used to make important organic molecules, such as bioactive natural products, pharmaceuticals, and agrochemicals. You will develop and increase your expertise in broad chemical synthesis and characterization techniques, whilst becoming familiar with the fundamentals of organic synthesis and photocatalysis. Furthermore, this project will require your collaboration with members of other research groups, thus improving your teamwork and networking skills. You will also develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: Ideally, you will already have skills and knowledge in general synthetic organic chemistry, analytical methods, teamwork and time management.

Bench fees: A bench fee of £10,000 is required.

How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

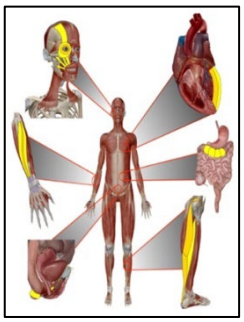
Supervisor: Your supervisor for this project will be Adam Noble, Research Fellow in the School of Chemistry. You can contact him at a.noble@bristol.ac.uk

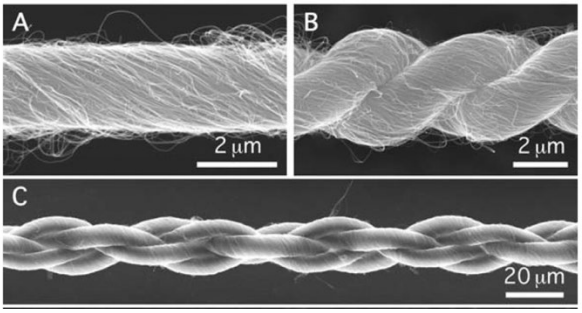
Find out more about your prospective research program: This review article provides an overview of ketyl radical chemistry, including different catalytic methods used for their generation:

Recent advances in the chemistry of ketyl radicals. *Chem. Soc. Rev.* **2021**, *50*, 5349 (https://pubs.rsc.org/en/content/articlepdf/2021/cs/d0cs00358a)

Empower – Artificial Muscles From Polymeric Architectures

About the project or challenge area: Muscles help us move, enable us to interact with objects and the environment, and regulate critical internal functions. Unfortunately, they are susceptible to damage due to disease, ageing and trauma and are a central factor in diverse serious healthcare conditions including sarcopenia (age-related loss of muscle mass and function, stroke, muscular dystrophy, multiple sclerosis, soft-tissue cancers, venous ulceration, diabetes, degenerative myopathy and incontinence). There are over 10.8 million people living with disability in the UK today. Nearly 6.5 million have mobility impairments, with the largest causes being age-related frailty and stroke (there are over 1.2 million stroke survivors in the UK). There is, therefore, significant demand for new treatments of muscle dysfunction, which will have significant global impact of the quality of life of many millions, with implantable medical devices steadily increasing for orthopaedic and diagnostic applications. In this project the aim is to explore the use of safe organic conducting materials, electrospun into fibers and yarns to form Twisted Electroactive Actuators (TEAs). The long-term goal for the development of TEAs will be to explore their use as implantable soft artificial actuators, to address the issues highlighted above.





Why choose this opportunity? The initial focus of your project will be on the preparation of electrospun electroactive polymer fibers which will provide an excellent platform to learn about the design of functional materials and their practical applications in the actuation process, meet the team and get acquainted with the laboratory. The secondary focus will be on the characterisation of the mechanical, electrical conductivity and biocompatiblity properties of spun and twisted fibers, giving you exposure to biocompatibility testing and consequent design, modification and optimization of materials properties. The final focus will be exploring the actuating properties of these novel TEAs, giving you experience in the Bristol Robotics Laboratory, as well as soft matter robotics in general. You will develop and increase your expertise in applied materials chemistry, whilst becoming familiar with the fundamentals of robotics, actuation and biocompatibility. Furthermore, this project will require your collaboration with other members across other research groups and Universities (both home and international), thus improving your teamwork and networking skills. You will also develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the large, international and dynamic Faul Research Group, who will provide support. You will also participate in the larger ongoing **emPOWER** project (working with clinicians, engineers, bioengineers and chemists). In addition, you will be assigned a student mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: Ideally you will already have skills and knowledge in electrospinning, polymer chemistry, soft matter actuators, biocompatibility testing, teamwork and time management.

Bench fees: A bench fee of £10,000 is required.

How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Charl Faul, Professor Chemistry in the School of Chemistry. Please see faulresearchgroup.com and @FaulResearch for further details. You can contact him at +44 (0) 117 954 6321 or email charl.faul@bristol.ac.uk

Find out more about your prospective research program: These articles explain the general background of twisted electroactive actuators:

Zhang et al, Science 306, 1358 – 1361 (2004)
Lima et al, Science 338, 928 – 932 (2012)
Chu et al., Science 371, 494–498 (2021)

Pioneering Novel Single Droplet Mass Spectrometry Tools to Investigate Aerosol Chemistry

About the project or challenge area: Atmospheric aerosols impact global climate directly by scattering sunlight and indirectly by serving as the seeds for cloud droplets. The aerosol indirect effect is the largest negative (i.e. cools the planet) and most uncertain radiative forcing. With respect to health, aerosols are a major component of air pollution. Chemical reactions in microscopic aerosols are complex: they can occur at rates much faster than in macroscopic solutions and have unique reaction intermediates and products relative to gas and aqueous phase reactions. However, few approaches exist to study the chemical composition of droplets >1 μm diameter.

The goal of this project is to develop new tools to study the surface and bulk molecular composition of microscopic droplets so that we can eventually investigate photochemistry at droplet surfaces. At Bristol we have already developed instruments (e.g. holographic optical tweezers and electrodynamic balances) to capture and study individual droplets in the size range of growing cloud droplets (~5-10 μm radius), providing information about droplet size, refractive index, surface tension, and viscosity. In this project, these tools will be coupled to a time-of-flight mass spectrometer by developing novel ionisation approaches to measure the molecular composition of individual picolitre droplets. Specifically, we will develop a voltage-free droplet assisted ionisation setup to measure the bulk composition of individual levitated droplets as well as a field-induced droplet ionisation setup to selectively measure the surface composition of levitated droplets. This research project will contribute to a major European Research Council funded grant aimed at investigating the surface composition of aerosols and their impacts on climate and health.

Why choose this opportunity? Aerosols are important to many aspects of our lives, including climate, air pollution, disease transmission, pharmaceutical interventions, and industrial formulations. The focus of this project is on developing new analytical technology. Although the primary application of this technology is in atmospheric chemistry, the approaches developed will be transferable to any domain where aerosols play a role. You will develop expertise in analytical and physical chemistry, particularly in the highly employable fields of mass spectrometry and aerosol science. The project will require collaboration across a team of individuals working on this and other related projects, along with collaborators across the globe. Your project will be aligned with the Centre for Doctoral Training in Aerosol Science, which hosts a reservoir of training materials in aerosol science and provides many networking opportunities. Furthermore, this project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. Additionally, you will be able to develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded within the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you identify any additional training needs or opportunities.

About you: Ideally you will already have skills and knowledge in analytical, physical, or atmospheric chemistry, teamwork and time management.

Bench fees: A bench fee of £3.5k is required.

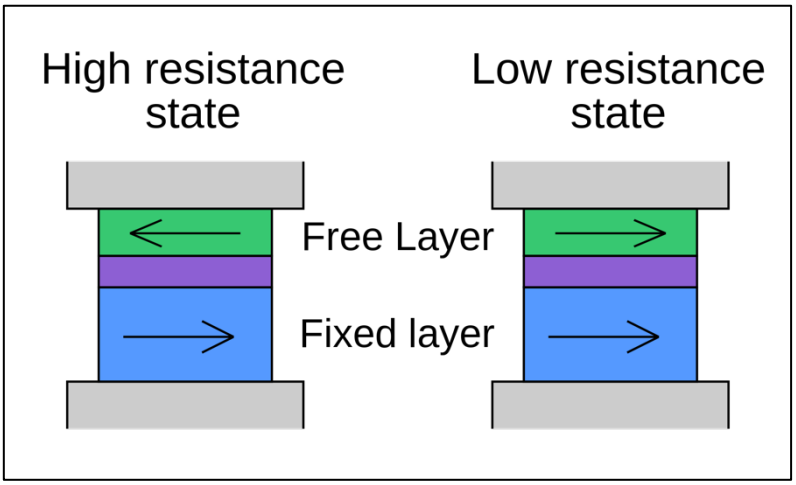
How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Bryan Bzdek, Proleptic Senior Lecturer in the School of Chemistry. You can contact him at b.bzdek@bristol.ac.uk.

Find out more about your prospective research program: For further background information on the analytical approaches to be developed, see these articles on droplet mass spectrometry: 1) Horan et al. *Analytical Chemistry*, **2017**, *89*, 1059-1062; 2) Grimm and Beauchamp, *Journal of Physical Chemistry B*, **2003**, *107*, 14161-14163. For further information on the Supervisor's recent research see the following publications: 1) Bzdek et al., *Communications Chemistry*, **2020**, *3*, 105; 2) Bzdek et al., *Proceedings of the National Academies of Science*, **2020**, *117*, 8335-8343.

A new material for improved electronics

About the project or challenge area: The most important challenge currently facing humanity is that of climate change. To help fight climate change, the UK has a target to achieve zero carbon emissions by 2050, but this will require a paradigm-shift in the way that energy is generated, supplied, used and stored. One of the first and most important steps we can take is to fast-track the development of green energy technologies that decarbonize our energy supply and facilitate the deployment of more advanced renewables. This objective is at the heart of the European Green Deal and in line with the EU's commitment to global climate action under the Paris Agreement. Research has suggested that there is a type of material that could generate spin-polarized current without perturbing the surrounding elements magnetically in a spintronics device. These so-called half-metallic antiferromagnetic (HM-AFM) materials were first predicted to exist in 1995, but have not of yet been produced experimentally. By acting as a spin valve, an HM-AFM material would be able to perform as a magnetoresistive switch in a very small, applied field and as such, enable more energy efficient fast switching.



Research at Bristol has shown that inorganic materials can be synthesized with exquisite control over composition, even up to quaternary and quinternary compounds. This immediately opens the opportunity to synthesize novel compounds and test them for the long-sought after HM-AFM behaviour.

Why choose this opportunity? The focus of your project will be on the synthesis of inorganic compounds which will provide a tremendous opportunity to learn about the design of functional materials and their performance as HM-AFMs. Your work in this area can make a real impact on the global challenge of climate change. You will develop and increase your expertise in sol-gel and solid-state syntheses and characterization techniques, whilst becoming familiar with the fundamentals of spintronics. Furthermore, this project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. You will also develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development. Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: Ideally you will already have skills and knowledge in general chemistry, and analytical methods, along with teamwork and time management.

Bench fees: A bench fee of £5,500 is required.

How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Professor Simon Hall, in the School of Chemistry. You can contact him via email - simon.hall@bristol.ac.uk

Find out more about your prospective research program: This recent article showcases our method of inorganic compound synthesis:

Facile synthesis of five strontium niobate metastable crystal compositions via sol-gel ionic liquid synthesis

https://doi.org/10.1016/j.ceramint.2021.01.285

Mechanisms of oxygen activation in biology

About the project or challenge area: Life in an aerobic environment requires activation of O_2. But activation of O_2 is thermodynamically unfavourable and requires electrons, which metalloenzymes can provide to control oxidative metabolism in biology. The catalytic capability of oxygen-activating iron enzymes is truly enormous and offers huge future potential for biocatalysis and biotechnology applications. The process works because, unlike other metals, a redox-active transition metal can change oxidation state and in doing so can push electron density onto a dioxygen (O_2) ligand (thereby "activating" the oxygen). In the presence of a suitable reductase, this leads to rapid cleavage of the O-O bond and the formation of a high-valent state, Fig. 1. It is this formation of high oxidation states that drives all metal-catalysed biological activation. In the case of iron, a high valent ferryl species is always used, Fig. 1. These ferryl intermediates provide the oxidative power for biological oxidations catalyzed by both non-heme and heme iron-containing enzymes. This project focuses characterizing the latter category.

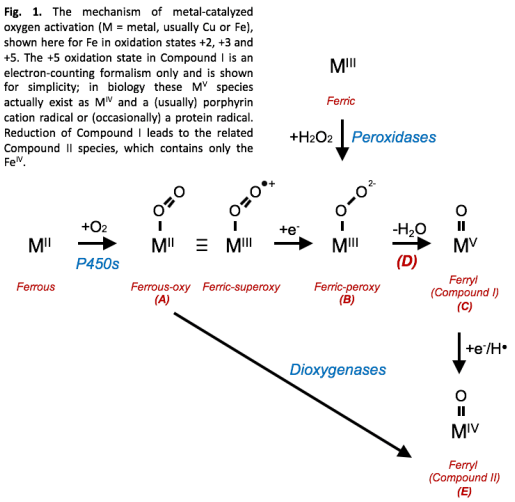
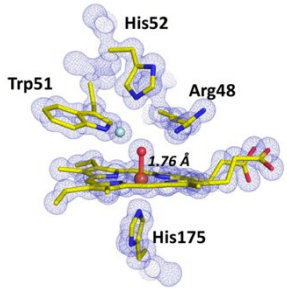


Fig. 1. The mechanism of metal-catalyzed oxygen activation (M = metal, usually Cu or Fe), shown here for Fe in oxidation states +2, +3 and +5. The +5 oxidation state in Compound I is an electron-counting formalism only and is shown for simplicity; in biology these M^V species actually exist as M^{IV} and a (usually) porphyrin cation radical or (occasionally) a protein radical. Reduction of Compound I leads to the related Compound II species, which contains only the Fe^{IV}.



Why choose this opportunity? There have many attempts to study the mechanisms of O-O bond cleavage in heme enzymes. But none of the previous methods can actually *visualise* the O-O bond cleavage steps – they can only access intermediates if they are stable enough, formed quantitatively and on the correct timescales. This means that a true visualisation of the O-O bond breaking steps has not been possible. In this proposal, we intend to shift the debate from the static – looking at static intermediates at single points in time – to the dynamic – visualising bond breaking and bond making events in real time. Serial femotosecond crystallography (as a collaboration with Prof A Orville, Diamond) provides a way forward because it allow us to access short lived intermediates formed during the O_2 activation event and on timescales that have not been previously accessible – in essence, building a molecular movie of catalysis. Since all heme enzymes use the same chemistry for O_2 activation, Fig. 1, the results generated will be generically relevant across all heme enzymes and will therefore be of wide impact. There are opportunities to work with structural biologists and beam line scientists around the world, who are interested in the dynamics of heme catalysis. You will participate with others in the group in external conferences (on-line), giving you an opportunity interact with other scientists outside of Bristol and to present your work to a wider audience. You will learn a range of techniques in chemical biology, enzymology, molecular biology and structural biology.

Full training will be provided for all aspects of this project. You will be embedded in the Prof Raven's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: You will have skills and knowledge in chemistry, chemical biology or biochemistry. You will be prepared to work well in a team, and be able to manage your time efficiently. These skills are desirable but not essential.

Bench fees: A bench fee of £7.5 k is required.

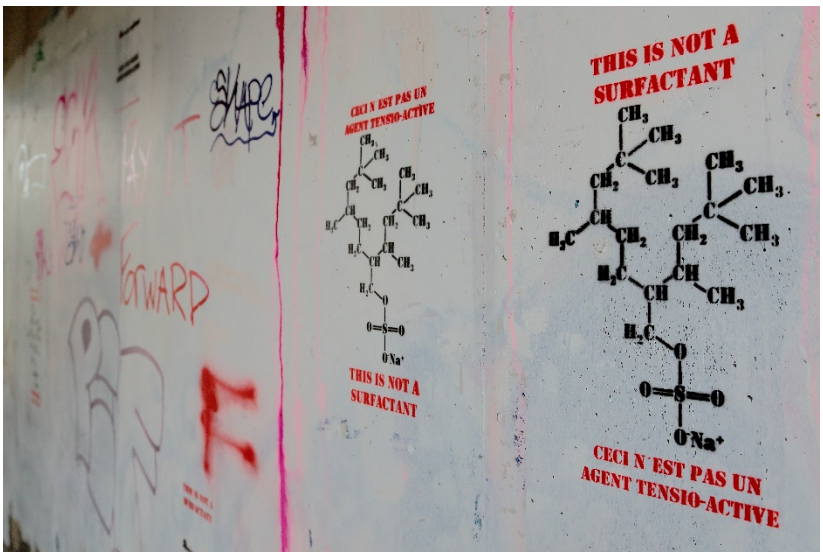
How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Your supervisor for this project will be Professor Emma Raven in the School of Chemistry. You can contact her at +44 (0) 117 928 7657 or email emma.raven@bristol.ac.uk.

Find out more about your prospective research program: Published work from the Raven lab below gives more information. *Science,* **2014***, 345*, 193-197 (DOI: 10.1126/science.1254398); *Proc. Natl. Acad. Sci USA* **2021**, 118 (22) 118 No. 22 e2104008118 (DOI: 10.1073/pnas.2104008118); Moody, P. C. E., Raven, E., *Acc Chem Res* **2018,** *51*, 427-435; *ACIE* **2020**, *60,* 1

New environmentally safe non-fluorinated surfactants for fire-fighting foams

About the project or challenge area: Certain surfactants and polymers contain fluorine, giving them desirable properties such as chemical and thermal stability, as well as high surface activity needed for stabilizing interfaces and foams. These fluorinated chemicals are known as perfluoroalkyl substances (PFAS), and because they do not breakdown they have been dubbed "forever chemicals". Hence, for sound environmental reasons, PFAS must be phased out. However, replacing these "forever chemicals" with fluorine-free analogues is easier said than done! Recent research at Bristol has shown how to attain the beneficial physical and chemical properties of fluorinated surfactants, but with newly designed molecules which are totally fluorine-free (see below).



Why choose this opportunity? The focus of your project will be on surfactants, polymers and colloid and interface science which will provide an excellent platform to learn about the design of functional materials and their practical applications. Your work in this area can make a real impact on global challenges, such as environmentally responsible fluorine-free surfactants for high volume applications such as waterproof coatings (e.g. Gore-Tex) and fire-fighting foams. You will develop and increase your expertise in broad chemical synthesis and characterization techniques, whilst becoming familiar with the fundamentals of colloid and interface science. Furthermore, this project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. You will also develop a range of transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: Ideally you will already have skills and knowledge in general preparative chemistry, analytical methods, and colloid science, teamwork and time management.

Bench fees: A bench fee of £5,500 is required.

How to apply: Applications are accepted throughout the Academic Year, and you should complete the online application form for Chemistry (MSc by Research).

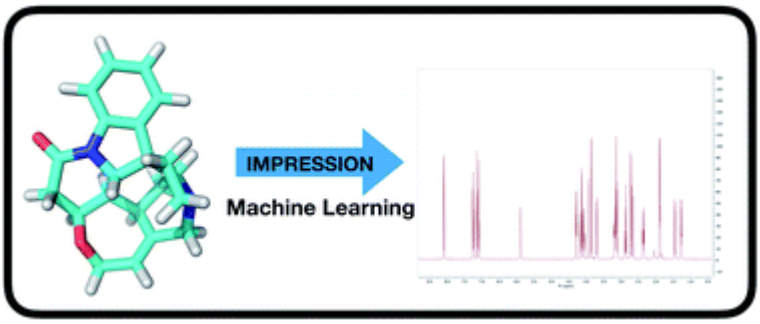
Supervisor: Your supervisor for this project will be Julian Eastoe, Professor Chemistry in the School of Chemistry. You can contact him at +44 (0) 117 928 9180 or email Julian.Eastoe@bristol.ac.uk

Find out more about your prospective research program: This review article explains the general background to fluorine-free surfactants:

Surfactants at the design limit
Langmuir, 2015, 31, 8205–8217
https://pubs.acs.org/doi/abs/10.1021/acs.langmuir.5b00336

Digital Chemistry – Machine learning, computation and chemical properties

About the project or challenge area: The project will develop new directions for our machine learning tool – IMPRESSION (see ref. below) – which predicts chemical/physical/spectroscopic/biological properties directly from 3D molecular structures. The first generation of IMPRESSION was used to predict NMR parameters with accuracies that approached quantum mechanical methods (such as Density Functional Theory – DFT), but hundreds of thousands of times faster. However, IMPRESSION Generation 1 was limited to prediction for molecules containing H, C, N and O only, used resource-heavy machine learning tools and could only predict NMR parameters. Recent results in our group suggest that IMPRESSION can applied to many other types of predictions, including ligand-binding efficiency (used in early-stage pharmaceutical development), solubility, acidity – pretty much any property that can be predicted by quantum mechanical methods. We have also developed a neural-network based approach which as the potential to deal with 1000-fold more classes of molecules, allowing us to move beyond H, C, N, O and into the entire range of relevant chemical space in the periodic table.



So we want you to explore this new world – building new generations of our IMPRESSION machine, building new datasets on which we can train it, and setting it new challenges to address.

Why choose this opportunity? The focus of your project will be on predicting chemical properties and behaviours using *machine learning and computational chemistry* which will provide an excellent platform to learn how computation and machine learning are applied to *modern chemical research problems*. Your work in this area can make a real impact on cutting edge scientific problems and global challenges, such as molecular design for drug development. You will develop expertise in *computational chemistry*, *coding* and *machine learning*, whilst becoming more familiar with the fundamentals of molecular structure and dynamics. Furthermore, this project will require your collaboration across research groups, including *synthetic chemists* and *spectroscopists*, and working our *industrial collaborators*, thus improving your teamwork and networking skills. You will be developing a range of additional transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: You will have skills and knowledge to understand the physical or chemical concepts behind molecular structure and chemical computation and an enthusiasm (but necessarily experience of!) coding and machine learning. You will enjoy working in teams and have good time management. These skills are desirable but not essential – what you don't have, we will teach you.

Bench fees: A bench fee of £5,500 is required.

How to apply: Applications are accepted throughout the year and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Craig Butts, Professor of Structural and Mechanistic Chemistry in the School of Chemistry. You can contact him at Craig.Butts@bristol.ac.uk

Find out more about your prospective research program: This article demonstrates our machine learning tools applied to property prediction (in this case NMR):

IMPRESSION – Prediction of NMR parameters for 3D Chemical Structures https://doi.org/10.1039/C9SC03854J

Exploring Atmospheric Photochemistry using Ultrafast Laser Spectroscopy

About the project or challenge area: Photochemical reactions are of vital importance in the natural world, and are exploited in many areas of science, technology, and medicine. For example, they initiate the mechanisms of animal vision, drive photosynthesis, affect air quality in our cities, and are central to advances in cell imaging using fluorescence microscopy. Photochemical reactions begin with absorption of light by molecular chromophores, leading to electronic and structural changes in the absorbing molecules. In natural and artificial systems, these chromophores are often surrounded by a complex environment such as an aqueous solution or a protein, with the surroundings playing a crucial role in controlling the photochemical outcomes. This research project will contribute to a major new EPSRC-funded programme of research *Ultrafast Photochemical Dynamics in Complex Environments* (EP/V026690/1, led by the University of Bristol) to explore how molecular-level interactions with the surrounding environment affect the photochemical pathways of molecules of environmental, biological, and technological importance. The project will apply transient absorption spectroscopy using the ultrafast laser system at the University of Bristol to study the photochemical changes that occur in aqueous solution for selected compounds of atmospheric importance. The three target molecules are glyoxylic acid, pyruvic acid, and 2,4-dinitrophenol. The outcomes will contribute to our understanding of how organic compounds in aqueous droplets oligomerize photochemically to produce secondary organic aerosol particles in ambient air.

Why choose this opportunity? A molecular-level understanding of photochemical processes is essential to address current challenges facing society, such as mitigating pollutants in air, developing new tools for disease diagnosis, sustainably improving crop yields, and efficiently harnessing solar energy. The focus of your project will be on atmospheric photochemistry, which will provide an excellent platform to learn about the environmental impacts of anthropogenic emissions. Your work in this area can make a real impact on global challenges, such as improving air quality in our cities, with benefits to the health of the population. You will develop and increase your expertise in spectroscopic and photochemical techniques, while becoming familiar with the fundamentals of molecular photochemistry and atmospheric chemistry. Furthermore, this project will require your collaboration with other research groups in Bristol and the partner Universities in the EPSRC-funded programme, thus improving your teamwork and networking skills, and giving you an opportunity to learn about how photochemistry is important in other scientific and technological areas. You will develop a range of additional transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world, learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: You will have skills and knowledge in physical chemistry, reaction kinetics, analytical methods, teamwork and time management. These skills are desirable but not essential.

Bench fees: A bench fee of £3000 is required.

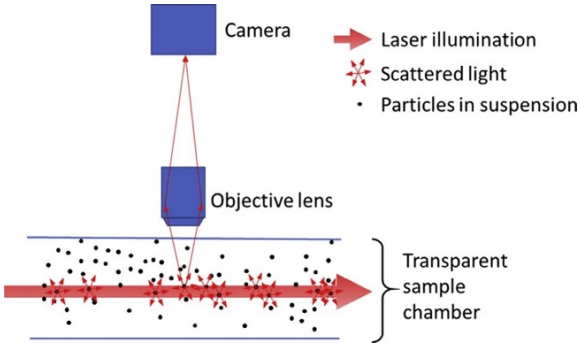
How to apply: Applications are accepted throughout the year, and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Andrew Orr-Ewing, Professor of Physical Chemistry in the School of Chemistry. You can contact him at +44 (0) 117 928 7672 or email a.orr-ewing@bristol.ac.uk

Find out more about your prospective research programme: For further background to the research field, see this article on the environmental photochemistry of α-keto acids such as pyruvic acid: Rapf *et al*., ACS Central Science 2018, **4**, 624. For information about the University of Bristol's laser spectroscopy and dynamics group, see www.bristoldynamics.com. Descriptions about the use of ultrafast laser spectroscopy to study photochemical dynamics can be found in recent publications from the Bristol group listed here: https://research-information.bris.ac.uk/en/persons/andrew-j-orr-ewing/publications/**.**

Enhancing Nanoparticle Tracking Analysis with deep learning

About the project or challenge area: Nanoparticle tracking analysis (NTA) has shown considerable promise for the reliable characterization of nanomaterials, in the fields of biopharmaceuticals, viral research, and protein aggregation. The figure illustrates schematically the NTA technique. A liquid sample containing nanoparticles (of diameters 10-1000 nm) is illuminated by a tightly-collimated laser beam. Light scattered by particles is collected by a microscope objective and imaged onto a camera. Tracking the Brownian motion over time yields the mean-squared displacement in two dimensions and, from the Stokes-Einstein equation, the size of multiple individual nanoparticles.



Although NTA provides highly-accurate sizes it suffers from a number of restrictions. First, NTA operates only within a relatively narrow window of particle concentration (~10^8 particles/mL) which means most samples require extensive dilution. This is because of a combination of laser brightness / camera sensitivity and the need to differentiate a particle from camera noise. We will explore how newly-developed deep learning techniques may be used to improve the robustness of the nanoparticle tracking algorithms, remove the need for subjective input, and so significantly extend the concentration regime over which NTA can be used. Second, it is difficult to reliably estimate nanoparticle concentrations with NTA because of a lack of knowledge of the depth of field within which the microscope is tracking particles and the need to compensate for edge effects. We will synthesize stable reference nanomaterials, with a certified number concentration of particles of different sizes and refractive indices, which can be used to accurately calibrate *in-situ* the NTA depth of field and so yield accurate particle concentration measurements. This will considerably extend the usefulness and applications of NTA.

Why choose this opportunity? The focus of your project will be on developing sophisticated physical measurement techniques and demonstrating how they can be improved using machine learning methods. The project will provide an excellent platform to learn about AI techniques, digital microscopy, scientific computing, and the characterization of nanoscale materials and their practical applications. NTA is currently being used to check the stability and manufacturing quality of COVID-19 vaccines so your work in this area can make a real impact on global challenges. In addition to physical and computing skills, you will develop and increase your expertise in broad chemical synthesis and characterization techniques, whilst becoming familiar with the fundamentals of nanoscience. This project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development. Full training will be provided in all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: You will have skills and knowledge in chemistry and a willingness to learn new skills in optics, microscopy and computation, where necessary. Full training will be provided.

Bench fees: A bench fee of £4000 may be required however we are currently in active discussions with a major UK instrument manufacturer who may make a contribution.

How to apply: Applications are accepted throughout the year and you should complete the online application form for Chemistry (MSc by Research).

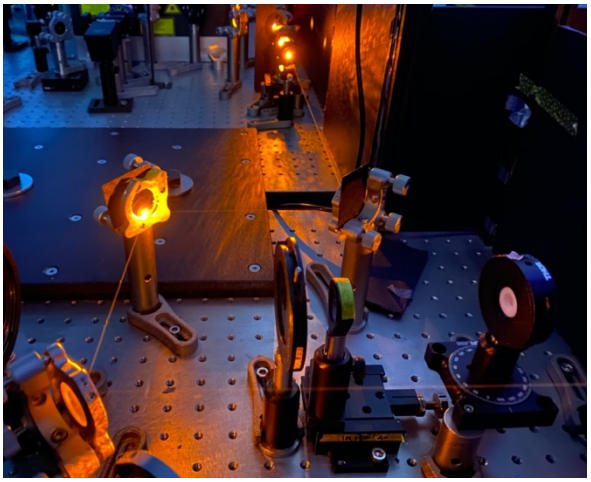
Supervisor: Your supervisor for this project will be Paul Bartlett, Professor of Soft Matter Science in the School of Chemistry. You can contact him at p.bartlett@bristol.ac.uk

Finding out more about your prospective research program: This recent article reviews recent work on NTA:

Kim, A., Ng, W. B., Bernt, W. & Cho, N.-J. Validation of Size Estimation of Nanoparticle Tracking Analysis on Polydisperse Macromolecule Assembly. *Scientific Reports* **9:2639**, (2019). 10.1038/s41598-019-38915-x

Investigating Molecule–Environment Interactions with Ultrafast Laser Spectroscopy

About the project or challenge area: Absorption of light by molecules initiates a fascinating correlated dance of electrons and nuclei that underpins many important photochemical reactions, such as the primary steps of photosynthesis or a *cis-trans* isomerisation that initiates vision. The outcomes of such photoinduced reactions are determined by how the electronic structure of constituent molecules changes by absorption of light, their time-dependent interactions (on femtosecond ($1x10^{-15}$ s) to picosecond ($1x10^{-12}$ s) timescales) with adjacent chromophores and rapid fluctuations of the surrounding environment. Using state-of-the art multidimensional optical spectroscopies (see link below) and tailored laser light pulse sequences we can take snapshots of an ensemble of thousands or millions of molecules at a time, and thus deduce the timescale and pathway(s) of energy flow between molecules in liquids or solids. From this vital information, we can derive the key inter-molecular interactions required for robust and efficient natural photochemical reactions and use this as inspiration for the next generation designer man-made chemical or protein systems. The project will involve looking at molecular interactions of chromophores in unusual solvents such as ionic liquids or inside model proteins that only incorporate a limited number of light absorbing molecules.



Why choose this opportunity? The focus of your project will be on photochemistry and ultrafast laser spectroscopy which will provide an excellent platform to learn about the fundamental molecular-level interactions of molecules with their environment. Your work in this area can make a real impact on global challenges solar energy capture and storage, by developing a greater understanding how molecules transfer energy between each, and the environment influences the outcome of the photochemical reaction. You will develop and increase your expertise in broad analytical skills and spectroscopic techniques, whilst becoming familiar with the fundamentals of ultrafast laser chemistry. Furthermore, this project will require your collaboration with other members across other research groups, thus improving your teamwork and networking skills. You will furthermore be developing a range of additional transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: You will have skills and knowledge in general physical chemistry, spectroscopic and analytical methods, data analysis, teamwork and time management. These skills are desirable but not essential.

Bench fees: A bench fee of £4000 is required.

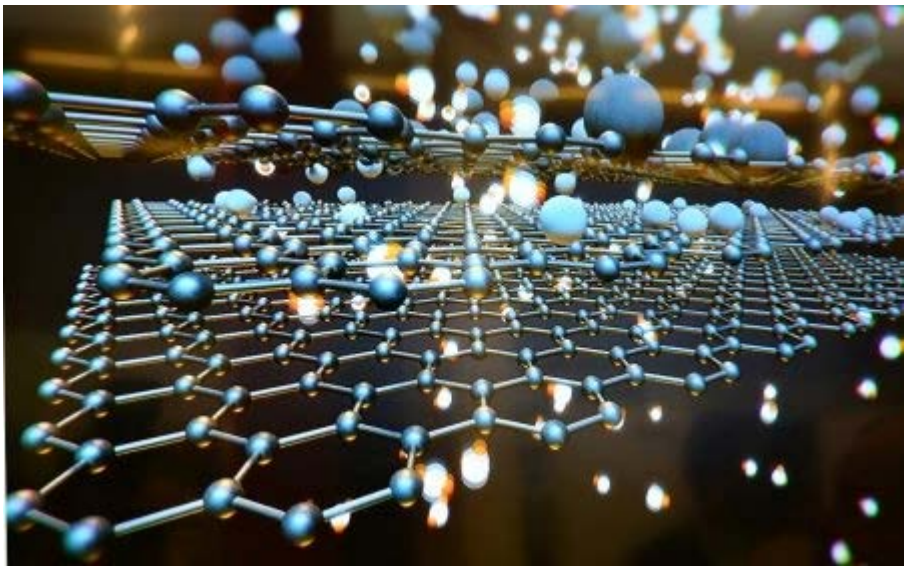
How to apply: Applications are accepted throughout the year and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Tom Oliver, Proleptic Associate Professor of Chemistry and Royal Society University Research Fellow in the School of Chemistry. You can contact him by email tom.oliver@bristol.ac.uk

Find out more about your prospective research program: This review article explains the unique aspects of multidimensional ultrafast laser spectroscopy:

Recent advances in multidimensional ultrafast spectroscopy, R. Soc. Open Sci., **5**, 171425 (2018). http://dx.doi.org/10.1098/rsos.171425

Molecules on graphene as functional nanocomposites



About the project or challenge area: Graphene, a two-dimensional monolayer of carbon atoms, has gained wide interests since its discovery. In many potential applications of graphene in bioanalytic devices and functional composites, it often comes into intimate contact with aqueous systems containing ions and bio(macro)molecules. Using X-ray reflectivity (XRR) at European Synchrotron Radiation Facility (ESRF, France), results from a Bristol MRes project has recently revealed the presence of a diffuse air-bubble layer on chemical vapor deposited (CVD) graphene when it is submerged in water. The air-bubble layer then diminished, and the graphene-water interface would become enriched with ionic species from the aqueous media. These unprecedent results have important implications to bioanalytic and nanotechnological applications of graphene in which its dynamic interfacial structure in contact with electrolyte solutions is crucial https://sciencetrends.com/vanishing-air-bubble-layer-and-ion-adsorption-on-graphene-in-aqueous-media/. This project will utilize quantitative state-of-the-art physicochemical methods, including neutron and X-ray scattering (at central facilities in the UK, France, and Germany), AFM and SEM imaging, to interrogate the interfacial structure at the graphene-water interface self-assembled from lipids and biomacromolecules.

Why choose this opportunity? Graphene is among the most exciting scientific discoveries of recent times, with immense potential for future exploitation as functional materials. The work in this area will advance our fundamental knowledge underpinning such potential. You will develop knowledge in fundamentals of graphene, lipids, biopolymers, nanocomposites, colloid and interface science. You will also develop expertise in quantitative physicochemical techniques, including synchrotron X-ray scattering. Our group is highly international and dynamic, with extensive industrial and academic links in the UK and worldwide. You will have the opportunity to interact and collaborate with the members across the group, developing transferrable skills. Specifically, we will have the opportunity to collaborate with a UK-based graphene manufacturer to implement your knowledge in real applications. Your professional and personal development, as well as enriching cultural experience, is central to the training programme. You will be supported throughout the project through individual and group meetings, graduate courses, and technical training, tailored to your specific needs. You are encouraged and supported to present your work at international conferences publish your work at international journals.

About you: Skills and knowledge in physics, materials, chemistry, analytical methods, and colloid science is desirable but not essential. Training will be provided.

Bench fees: A bench fee of £4000 is required. A small number of School of Chemistry Bench fee bursaries are available to part-cover bench fees

How to apply: Applications are accepted throughout the year and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Dr Wuge Briscoe, Reader in Physical Chemistry in the School of Chemistry. You can contact him at +44 (0) 117 3318256 or email wuge.briscoe@bristol.ac.uk

Find out more about your prospective research program: "2010 Nobel Physics Laureates" (PDF). nobelprize.org; *Graphene surface structure in aqueous media: Evidence for an air-bubble layer and ion adsorption* https://doi.org/10.1016/j.carbon.2018.10.093; *Surface structure of few layer graphene* https://doi.org/10.1016/j.carbon.2018.04.089