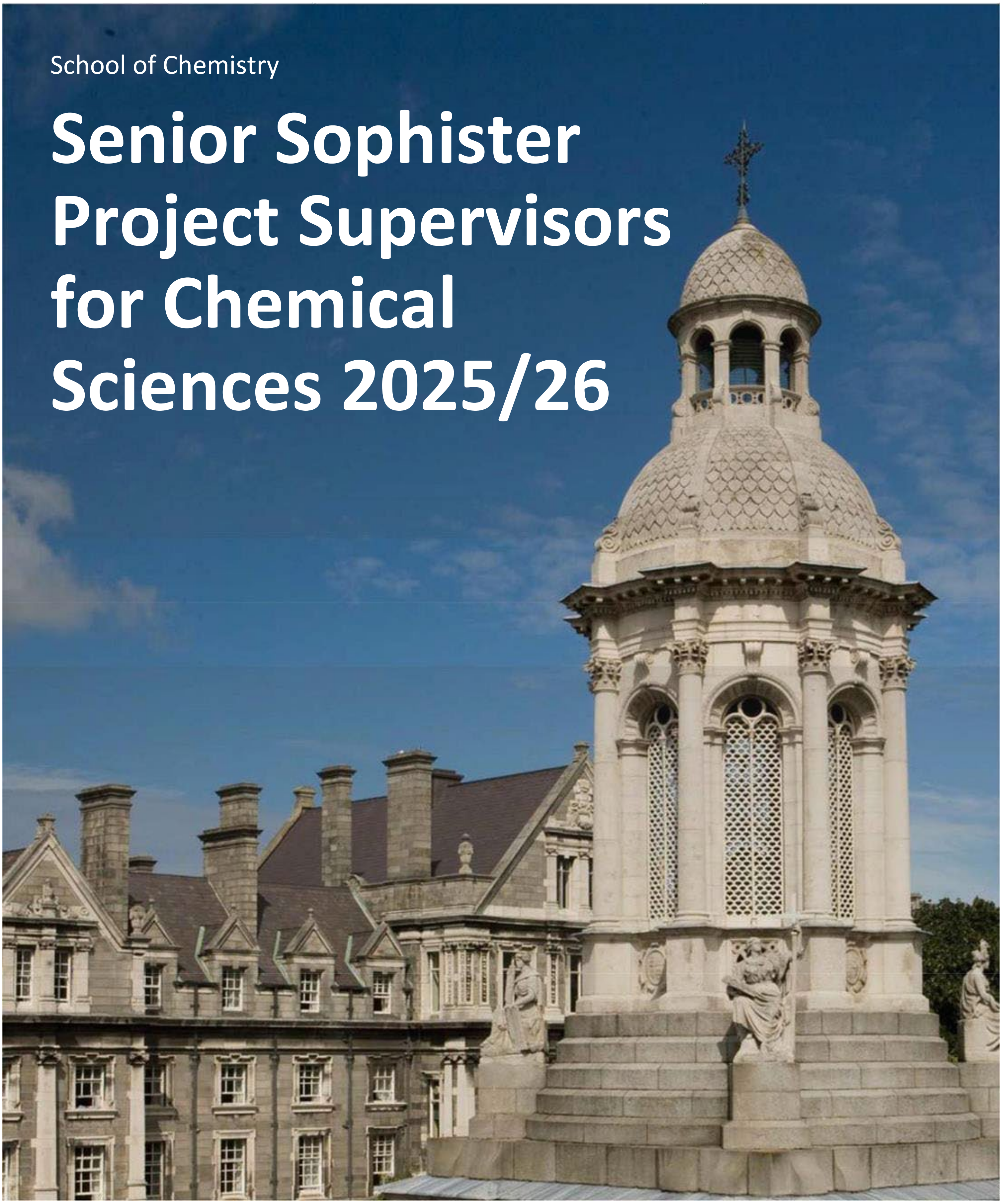
Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

School of Chemistry

Senior Sophister Project Supervisors for Chemical Sciences 2025/26



Contents

Inorganic and Synthetic Materials Chemistry Based Projects

Prof. Robert Baker
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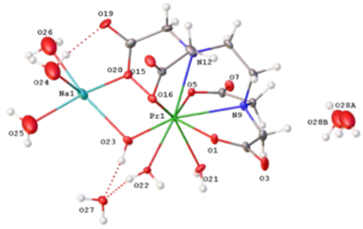
Discipline: Inorganic chemistry

Areas of Research (Keywords): f-block chemistry, homogeneous catalysis, supramolecular chemistry, radiochemistry

Summary of type of research projects that could be undertaken:

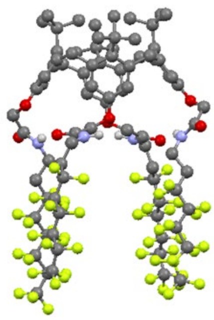
The Baker group have their roots in the underexplored chemistry of the f-block, both lanthanides and actinides. We are also interested in designing new ligands for lanthanide separation (for WEEE applications) using a supramolecular approach and incorporating lanthanides as catalysts in plastics that can then be 3D printed.

1. Lanthanide chemistry: With the correct choice of ligands we can manipulate the redox potentials of the lanthanide ion to stabilise unusual oxidations states and we are targeting Pr(IV) and Tb(IV) of which there are only a few examples (J. Am. Chem. Soc. 2020, 142, 5538–5542). This project would entail air sensitive chemistry, ligand synthesis and X-ray diffraction.



2. 3D printed catalysts: We have recently shown that we can incorporate transition metals and lanthanides into commercially available plastics and 3D print labware. In this project you would expand this process to industrially relevant catalytic applications.

3. Lanthanide separation: We have designed ligands that rely on outer sphere hydrogen bonding to quantitatively extract gold from acidic solutions. In this project you will expand on this concept to the technologically relevant lanthanide ions where the donor ligands can be modified and the fluorinated ponytails allow physisorbtion onto Teflon tape so a very simple methodology of lanthanide removal could be developed. In this project you will conduct fluoro-organic synthesis and advanced characterisation techniques to quantify the amount of Ln sorbtion.



*We are not able to offer modelling/computational-type work for potential CMM students.

Prof. Colm Delaney
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Discipline: Inorganic and Materials

Areas of Research (Keywords): self-assembly, colloidal nanoparticles, liquid crystals, direct laser writing, spectroscopy, sensing, encryption

Summary of type of research projects that could be undertaken:

Self-assembly is a spontaneous process which can reversibly form structures from the molecular scale to the mesoscale. These reversible processes can be controlled and exploited by molecular design, enthalpic/entropic contributions, particle size and design, the environment that separates particles, and the driving forces which promote structure formation. Direction and control of self-assembly would serve to bridge the void between chemical synthesis on the molecular level, and manufacturing on the macroscale. Our group exploits self-assembled materials, and the processes which form them, to create controllable biomimetic structures, like the ones nature has optimised to signal, harvest light, camouflage, or collect water. We then apply these structures in photonics, tissue engineering, sensing, and microelectronics.

For Capstone students, research projects could involve the synthesis of a selection of self-assembling functionalised nanomaterials, such as silica and polymer nanoparticles, cellulose nanocrystals, photoactive azobenzene nanoparticles, or even liquid crystals. While varying shape, size, or surface charge, students would fully characterise the nanomaterials using NMR, AFM, SEM, TEM, DLS, and zeta potential. In the Delaney group we are developing means of precisely altering inter-particle distance in the 3D superlattice post self-assembly to access spacings and periodicities currently precluded by the thermodynamics of self-assembly. Such control is significantly beneficial for the advancement of self-assembled nanoparticle/nanocrystal systems in photonics, plasmonics, biosensing, and data storage.

For students who enjoy numerical simulation, a series of more complex material architectures could be created, which combine intrinsic and extrinsic ordering. Finite difference time domain simulations would then be used to model the nanoparticle ordering, and to predict the effect of both the ordered nanomaterials and surface nanostructures.

For students who are interested in chemical/physical sensing or encryption, microstructures fabricated from functionalised nanoparticles would be incorporated into microfluidic devices and their response probed using optical microscopy, micro-spectroscopy, nanoindentation, SEM imaging, and Raman-AFM, under external stimulus. Students would also have the opportunity to work on developing scripts to generate machine-learning code for automatic spectral analysis of micropixel sensor arrays within tissue-engineering models.

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Prof. Sylvia Draper

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Discipline: Inorganic and Materials Chemistry

Areas of Research (Keywords): Organic/Inorganic Synthesis, Luminescent materials, Molecular graphenes, Anticancer therapeutics.

Summary of type of research projects that could be undertaken:

The Draper team identifies new designs and explores novel synthetic routes to polyaromatic compounds or ligands. Their goal is to create systems that demonstrate unusual and highly desirable material or photophysical properties. As a consequence of their work new strategies to develop strongly absorbing metal complexes with long-lived highly emissive excited states have emerged. These materials show improved performance as triplet photosensitisers (PSs) in triplet-triplet annihilation upconversion (TTA-UC), and generate singlet oxygen and Reactive Oxygen Species (ROS) that give rise to targeted cell death in photodynamic therapy (PDT) applications.

Two recent highlights are the formation of novel coordination complexes incorporating (i) ethynynl Nile Red chromophores and (2) non-symmetric bipyridines. The former possess non-emissive or 'dark' triplet states that can be used for singlet oxygen sensitising and for killing cancer cells at very low concentrations. The latter exhibit solvent-dependent excited state behaviours. Both these phenomena are rare and open-up a myriad of new opportunities for exploitation e.g. as sensors or as dual therapeutic agents.

Students working in the Draper Team gain experience in the synthesis of materials using Schlenk line, microwave and/or mechanochemistry techniques. They work in a dedicated team using specialist equipment that allows them to optimise their molecular designs and synthetic routes and in particular to exploit the opportunities offered by Green Chemistry methods. They learn how to purify and separate materials using sublimation, fractional crystallisation, thin layer and automated chromatography. In addition they learn to be comfortable applying a range of characterisation and spectroscopic techniques from IR, NMR, UV/Vis absorption/emission spectroscopy, to Cyclic Dichroism, Mass Spectrometry and electrochemistry.

Nationally the Draper team collaborates with John Colleran in TUD, Mary Pryce in DCU and Eoghan McGarrigle/Susan Quinn in UCD. You can expect to visit and gain access to the facilities in these groups/institutions.

*We are not able to offer modelling/computational-type work for potential CMM students.

References:

1. C Condon, R Conway-Kenny, X Cui, LJ Hallen, B Twamley, J Zhao, S.M.Draper, Journal of Materials Chemistry C 2021, 9 (41), 14573-14577 https://doi.org/10.1039/D1TC02830H
2. L Hallen, AM Horan, B Twamley, EM McGarrigle, SM Draper, Chemical Communications 2023, 59 (3), 330-333 https://doi.org/10.1039/D2CC04910D

Prof. Peter Dunne
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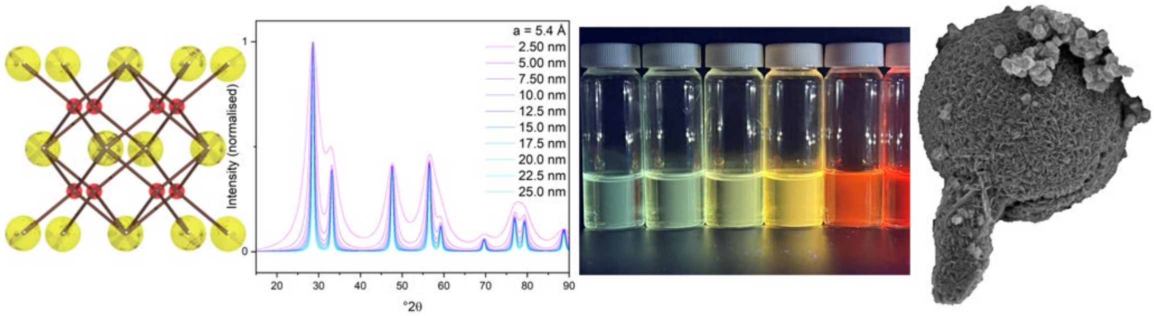
Discipline: Inorganic and Synthetic Materials

Areas of Research (Keywords): Materials Synthesis; Green Chemistry; X-ray Diffraction



Summary of type of research projects that could be undertaken:

Our research is focussed on the development of cleaner, greener, synthetic routes to functional inorganic nano- and micromaterials; including transparent conducting oxides, magnetic nanoparticles, quantum dots and bio-derived carbon dots; as well as broadening our understanding of material formation in non-conventional reaction conditions and biomimetic materials synthesis.
Synthetic methodologies include sol-gel, hydro/solvothermal reactions, novel solvent systems, and combustion syntheses using a mix of equipment from off-the-shelf reactors to custom, in-house designed and built apparatus.
Materials characterisation is performed by powder X-ray diffraction and Rietveld refinement using a new X-ray suite based in SNIAM; UV-vis, fluorescence, IR and Raman spectroscopies, as applicable; and Scanning and Transmission Electron Microscopy at the Advanced Microscopy Lab. These characterisation techniques may be coupled with statistical analysis methods, such as Principal Component Analysis, for rapid interpretation of large datasets.
Potential applications of the targeted materials include environmental remediation, catalysis, smart coatings, optics, biomedical imaging, and solar energy generation.

We collaborate with Profs. Baker, Delaney, and McAuley across these various research areas.

*Data analysis projects may be offered, but no molecular modelling.

Prof. Larisa Florea

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Discipline: Inorganic and Materials Chemistry

Areas of Research (Keywords): Polymer Chemistry, Hydrogels, Stimulus-response, Micro-actuators, Micro-fabrication

Summary of type of research projects that could be undertaken:
As the future of surgery is increasingly moving towards minimally-invasive, precision intervention, embracing microrobotic technologies in the realm of microsurgery holds great promise for the future of medicine. Progress towards realising breakthrough developments in the area of microrobotic tools must involve new strategies, and adoption of new materials, rather than incremental improvements in traditional engineering-based technologies.

Research in the **Florea group** (florealab.com) combines fundamental material synthesis, polymer science and microfabrication technologies, to provide access to 'adaptive' materials that switch between different states in response to various external stimuli. Stimulation of these materials using light, temperature, electrochemical potential, or changes in the local chemical environment can result in highly precise 4D control, from the nano- to the micro- to the macro-scale. The incorporation of responsive units at the molecular level, combined with precise assembly at the nano-/micro- level *via* controlled polymerisation methods, 3D design and micro-fabrication, permits the realisation of customised 3D architectures which can undergo anisotropic and directional/programmable shape change upon stimulation. Such microstructures have a wide range of applications, from soft micro-robotics to microfluidics and medical devices.

Research Areas
The projects available in the Florea group focus on **fundamental materials research** for addressing real-world challenges. Through multidisciplinary approaches, combining **chemistry, materials science, nanotechnology and 3D fabrication technologies**, we focus on the development of stimuli-responsive actuators, that respond to a variety of stimuli, such as light, electric or magnetic fields, or a change in the local environment. The aim of our research is to investigate the feasibility of using responsive polymers as micro-machines, capable of doing mechanical work in response to chosen stimuli. Moreover, new functionalities such as **sensing, and switchable uptake and release of molecular guests**, will also be incorporated in the same material, in order to create synthetic units with biomimetic features.

Opportunities for Students
We offer **experimental projects** in the area of **polymer chemistry**, involving synthesis and characterisation. During the projects the students will gain knowledge and experience in polymerisation protocols, photolithography and microfabrication alongside a wide range of materials characterisation methods such as SEM, FT-IR and RAMAN spectroscopy, solution-state and solid state NMR, confocal and STED microscopy, atomic force microscopy, among others.

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Prof. Y.K. Gun'ko
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Discipline: Inorganic Chemistry

Areas of Research (Keywords):
Nanomaterials, quantum dots, multimodal magnetic nanoparticles, carbon nanomaterials, 2D nanomaterials, chirality at nanoscale, bio-nano-technology, synthetic inorganic chemistry.

Summary of type of research projects that could be undertaken:

Our research explores the cutting edge of nanomaterials, inorganic chemistry, and nano-biotechnology, with applications spanning photonics, biomedicine, and advanced materials science. We focus on designing and optimizing functional nanostructures to address critical challenges in technology and healthcare.

Projects could involve the synthesis, characterization, and functionalization of semiconductor quantum dots for use in optoelectronics, biological imaging, and sensing. Researchers may explore ways to improve quantum dot stability, quantum efficiency, and biocompatibility. Another area of our research includes the development of multimodal magnetic nanoparticles for drug delivery, hyperthermia cancer therapy, and MRI contrast agents. Research may focus on tailoring surface chemistry for targeted delivery or optimizing multimodal magnetic properties for enhanced imaging. Investigations may focus on 2D nanomaterials such as boron nitride and graphene, or hybrid nanocomposites for applications in flexible electronics, energy storage, and high-performance materials. Researchers could develop new functionalization strategies to improve mechanical, electrical, or thermal properties. Projects may explore noncatalytic systems and membranes for environmental and industrial applications, including water purification, pollutant removal and carbon dioxide capture and conversion.

Our projects are inherently interdisciplinary, integrating synthetic chemistry, advanced spectroscopy, nanofabrication, and electron microscopy, providing diverse and exciting research opportunities for students passionate about chemistry, materials science, and bio-nanotechnology.

(Exact project title will be decided following discussion between supervisor and student)

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Prof. Aidan McDonald

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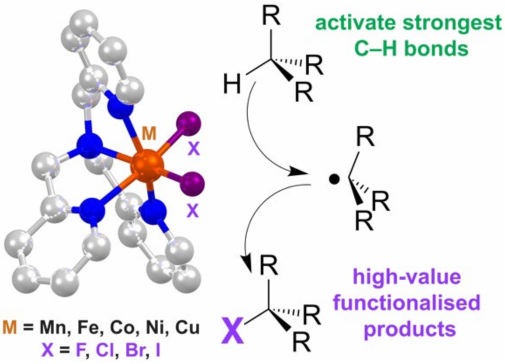
Discipline: Inorganic Chemistry

Areas of Research (Keywords): Synthetic Inorganic Chemistry, Oxidation Catalysis, Bioinorganic Chemistry, Transition Metal Chemistry

Summary of type of research projects that could be undertaken:

Project area 1: *High-Valent Oxidants:* The mild, cheap, and selective activation of hydrocarbons (for use in the pharmaceutical and agriculture industries) is a grand chemical challenge due to the strength of the C–H bond. The McDonald lab develops methods for bioinspired metal-mediated oxidative activation of C–H bonds in hydrocarbon substrates. We have identified that tuning of the reactivity of high-valent oxidants can be achieved by simple ligand exchange at high-valent oxidants. You will explore a new class of hydrocarbon oxidation reaction (using metal-halide oxidants), which we believe will achieve facile C–H activation under ambient conditions. Your main objective is to prepare metal-halides that are capable of activation and halogenation of the strongest of C–H bonds.



Project area 2: *Understanding Natural Photosynthesis:* Understanding the oxidative processes involved in solar energy capture in photosystem II (PSII) remains a challenging. Nature has evolved to perform these processes efficiently through the capture of solar energy, the splitting of water, and the generation of chemical fuels (O_2 and carbohydrate). We have limited understanding of the active oxidant in PSII (called $P680^+$). Our objective is to cultivate a fundamental understanding of the most potent oxidant in biology ($P680^+$). Specifically, you will prepare and characterise synthetic mono- or dimeric porphyrin complexes that mimic $P680^+$. You will investigate the factors that control the redox potential of these mimics to gain a thorough understanding of $P680^+$.

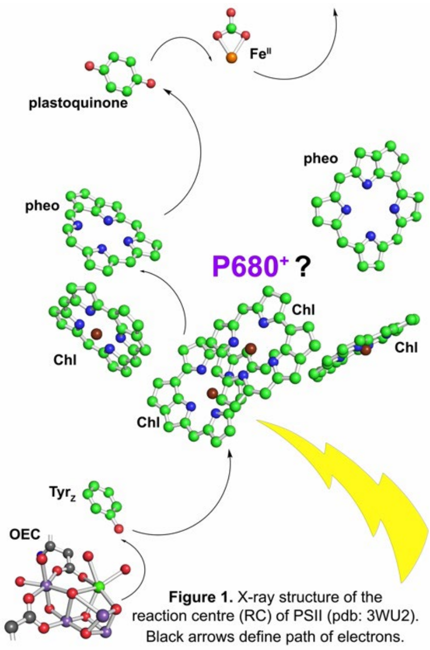


Figure 1. X-ray structure of the reaction centre (RC) of PSII (pdb: 3WU2). Black arrows define path of electrons.

During a Senior Sophister project in the McDonald lab, you will gain experience in synthetic organic and inorganic chemistry, anaerobic preparation techniques, catalysis, and NMR, EPR, Infra-red spectroscopy, electrochemistry, and mass spectrometric analysis.

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Prof. M A Morris

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Discipline: Inorganic

Areas of Research (Keywords):

Sustainability, materials chemistry, low carbon footprint, surface coatings, circular economy

Summary of type of research projects that could be undertaken:

Life cycle assessment of glass versus plastic (computation)

Plastic has a high environmental impact and is of limited circularity. Glass has a lower environmental footprint especially if it can be strengthened. This project is around quantifying the advantages of glass versus plastic.

Synthesis of nanofluids based on dielectric oils

Batteries (e.g. lithium ion-based systems) are limited by operational and charging temperatures which can lead to lower performance and shorter life of batteries. Increasing cooling by immersion into an oil can increase heat transfer allowing cooling and optimum use. However, heat transfer in oils is low but can be increased by addition of solid particles. This project will look at the synthesis of functionalised particles to allow more efficient cooling.

Membrane synthesis from used polymers

Polymer membranes are expensive materials using virgin polymers and solvents. However, waste plastics could be used to synthesise many polymers by solvation. This project will target the synthesis of PVDF (polyvinyl difluoride) membranes to avoid the manufacture of PVDF, a material that has been listed as a control substance in the EU.

Eco-friendly fertilizers

In order to maintain the presence of ammonia based fertilizers in the soil and the slow release of nutrient allowing less fertilizer to be used in crop production, a polymer film can be applied to fertilizer pellets. This can lead to production of microplastics. Here we will explore the use of wood derived polymers (lignin, cellulose etc.) which are biodegradable and can allow controlled release of the nutrient.

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Prof. Wolfgang Schmitt
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Discipline: **Inorganic & Materials Chemistry**

Areas of Research (Keywords): **Sustainable Energy; Carbon Capture; Hydrogen Generation; Coordination Chemistry; Supramolecular Chemistry; Metal-Organic Frameworks (MOFs); Devices; Light-Active MOFs**

Summary of type of research projects that could be undertaken:

Metal-Organic Frameworks and Supramolecular Coordination Cages for Sustainable Energy Applications, Catalysis and Bio-Medical Applications: Metal-organic frameworks (MOFs) and related coordination cages are important metallo-supramolecular materials, consisting of metal clusters or ions linked by organic ligands to form microporous networks or defined cavities. MOFs and related materials are regarded as key compounds in synthetic chemistry and materials science, as their unprecedented surface areas and associated modular synthetic concepts make them promising materials for various applications.[1] Students can choose from several interdisciplinary research projects focusing on the synthesis, characterisation, and functional applications of MOFs and molecular cages, with potential uses in: **(a) catalysis** (e.g., H_2 generation and other energy conversions), **(b) atmospheric CO_2 capture and/or CO_2conversion**, **(c) drug delivery**, and **(d) magnetic applications. (e)** A further area of interest is the design of **light-active MOFs** that mimic biological enzymes for **solar-fuel applications**.[2]

Each project can provide hands-on experience in synthetic chemistry, structural analysis (X-ray diffraction), electrochemistry, and functional material applications. Depending on the application area, research may involve multi-step organic and inorganic syntheses, characterisation techniques such as NMR &IR spectroscopy, single crystal X-ray diffraction, investigation of guest-host interactions for drug delivery, catalysis, or sensing. Additionally, students may work on MOF-based electrodes, assessing their performance in electrochemical/photoelectrochemical processes (e.g., H_2 evolution, CO_2 reduction).

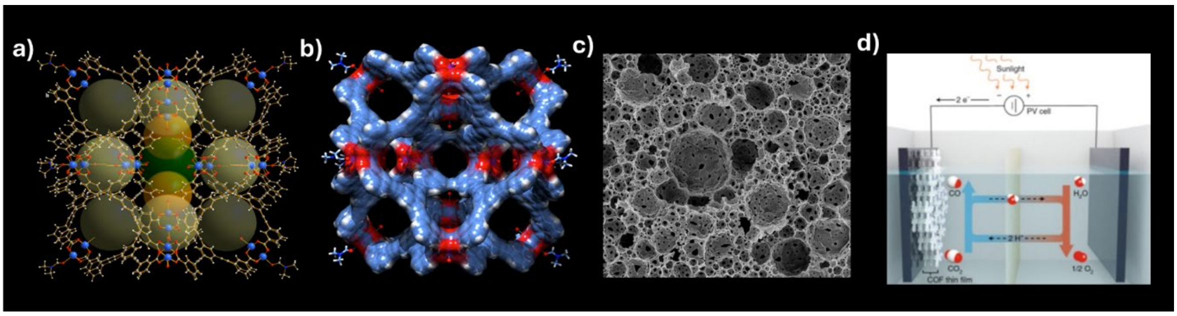

Figure 1. a) and b) Structure and topological representations of a coordination cage with exceptional cross-sectional diameters consisting of 36 Cu(II) ions and 24 organic ligands (see. Schmitt et. al. Nature Communications, 2017, DOI:10.1038/ncomms15268); c) Electron micrograph of a MOF deposited on an electrode highlighting its porous nature; d) Use of for MOF/electrode for the electrochemical reduction of CO_2 and for the oxidation of water.

References: [1] a) Furukawa et al., *Science* **2013**, *341*, 1230444; b) Diercks et. al. *Nature Materials* **2018**, *17*, 301; c) M. Yoshizawa et al., *Angew. Chem. Int. Ed*. 2009, *48*, 3418; [2] Selected relevant publications from the research group: a) Schmitt et. al., *Nature Communications*, **2024**, *15*, 10180; b) Schmitt et. al., *Chemical Science*, **2023**, *14*, 13722; c) Schmitt et. al., *ACS Sustainable Chemistry & Engineering*, **2020**, *8*, 13648; d) Schmitt et. al. *Nature Communications*, **2017**, 15268; e) Schmitt et. al., *Chemical Communications*, **2019**, *55*, 5013; e) Schmitt et. al., *Inorganic Chemistry,* **2019***, 58,* 19766.

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Organic, Medicinal and Biological Chemistry Based Projects

Prof. Stephen Connon

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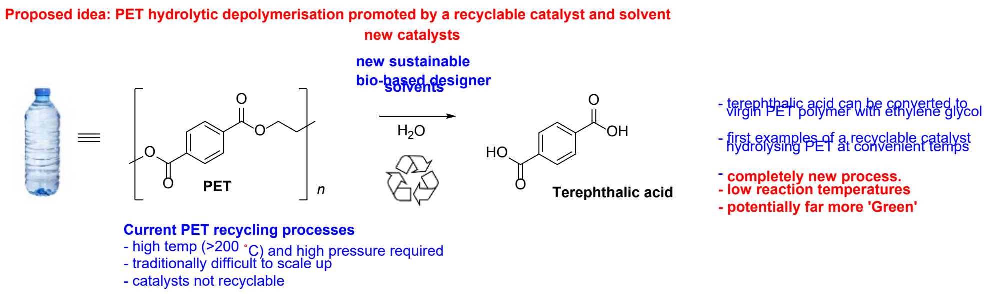
Discipline: Organic, Medicinal and Bioorganic Chemistry

Areas of Research (Keywords): plastic recycling, catalyst design, green chemistry



Summary of type of research projects that could be undertaken:

Polyethylene terephthalate (PET) is a plastic used in drinks bottles, packaging and textiles. In 2021, a staggering average of **>700 kg of this material was synthesised very second**.[1] The long half-life of these materials in the environment and their origins from fossil fuels are actively contributing to the current climate and ecological emergency; in addition to diverting existing fossil-based resources from more critical applications. Remarkably, most recycling of PET is physical in nature. The waste is of inferior quality to virgin polymer, so it is washed and reduced in size, then mixed with virgin polymer to make new 'recycled bottles'. Much less widespread chemical recycling[2] processes hold considerably greater potential from an efficiency standpoint – *e.g.* the depolymerisation of PET to a monomeric solid which can be repolymerised to new virgin polymer of high purity and quality.[3] Cleavage of the ester bonds in PET using water (the cheapest, safest and 'greenest' of solvents) is one such attractive methodology – however the plastic is insoluble in water and consequently most of these processes require high pressure apparatus and temperatures exceeding 200 ˚C. We have recently discovered completely new methods for hydrolysing either PET at lower temperatures in alkaline conditions below 100 ˚C in 3 h using novel catalysts, or at 138 ˚C in just 4 min.[4]

While these methods are either comparable or faster to current industrial processes – the holy grail is to be able to **depolymerise plastic rapidly at low temperatures with minimal waste**. This is beyond the scope of current technology. In order to achieve this, the use of co-solvents are required. Co-solvents have been used in the literature, but often the solvents are of environmental concern (e.g. dichloromethane,[5] THF) and/or are too expensive to be used on the massive scales that will be required to alleviate the future challenges associated with PET recycling. This project aims to develop completely new, bespoke **recyclable** solvents from biomass sources, and use them in tandem (for the first time) with powerful yet sustainable catalysts designed in our group to achieve the first efficient, low waste recycling of PET. This is quite a challenge which has never been attempted before – these will not be solvents in the traditional sense - we will use synthetic organic chemistry to modify biomass feedstocks to develop sustainable, **functional** solvents which can be recycled, mix with water, but also have an affinity for the PET and **actively work together with the catalyst**, so that reaction is rapid. This would suit a student with an enthusiasm for developing 'greener' reactions and an interest in making functional molecules that do things. This is a real frontier: over the last two years SS students working on PET recycling contributed to work being submitted for 4 publications and 3 patents.

References

1. https://plasticseurope.org/knowledge-hub/plastics-the-facts-2022/ (accessed 23/01/25)
2. A. H. Tullow, Plastic has a problem; is chemical recycling the solution? *Chem. Eng. News* **2019**, *39* https://cen.acs.org/environment/recycling/Plastic-problem-chemical-recycling-solution/97/i39i39 (accessed 03/01/25)
3. Reviews: a) E. Barnard, J. J. R. Arias and W. Thielemans, *Green Chem*. **2021**, *23*, 3765; b) S. C. Kosloski-Oh, Z. A. Wood, Y. Manjarrez, J. P. de los Rios and M. E. Fieser, Mater. Horiz., **2021**, *8*, 1084; c) P. Benyathiar, P. Kumar, G. Carpenter, J. Brace and D. K. Mishra, *Polymers* **2022**, *14*, 2366.
4. For recent work by our group in the area see: a) D. Bura, L. Pedrini, C. Trujillo and S. J. Connon, *RSC Sustain.* **2023**, *1,* 2197; b) L. B. Anderson, C. Molloy, L. Pedrini, I. L. Martin, S. J. Connon, *Green. Chem*. **2024**, *26*, 11125; c) I. L. Martin, L. B. Anderson, D. A. McAdams, C. Molloy, P. W. Dunne, S. J. Connon, *Chem. Commun*. **2025**, 61, 2750; d) L. Pedrini, C. Zappelli, S. J. Connon, *ACS Sustainable Chem. Eng*. **2025**, *13*, 1424.
5. H. Chen. H. Hu, *Ind. Eng. Chem. Res*. **2023**, *62*, 1292

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Prof. Thorfinnur Gunnlaugsson

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Discipline: Organic

Areas of Research (Keywords): Supramolecular and medicinal chemistry, organic chemistry, inorganic and coordination chemistry, functional materials, self-assembly and spectroscopy.

Summary of type of research projects that could be undertaken: My research group is engaged in the development of novel organic ligand structures, and their application in range of functional chemistries. This involves, the formation of luminescent and colorimetric sensors and imaging agents for use in chemical biology and medicinal chemistry, and the formation of novel ligands for use in coordination chemistry for both *d*- and *f*-metal ions. The latter we have used extensively in recent times to form self-assembly structures for range of applications, such as in the formation of functional devices. We have strong interest in the development of range of supramolecular structures and supramolecular materials, such as polymers, luminescent materials, coordination polymers and porous organic material, *etc*.

A typical SS project would be interdisciplinary in its nature, where the student would be engaged in organic synthesis, and when appreciate, in coordination chemistry. Carry out extensive characterisation of both the organic structures, the coordination complexes/polymers, and investigate the application of the systems developed. As such, each student is subjected to range of characterisation techniques and has the possibly to engage in topical research projects in close collaboration with dynamic team of researchers. The TG group has a well-equipped synthetic laboratory located in the TBSI building, fitted with equipment to carry out modern synthetic chemistries, as well as a dedicated instrumental laboratory, which hosts range of spectrometers. Each SS student will be fully integrated into the TG research group, and as such expected to experience all aspects of laboratory research and management, they will be trained in data analysis, such as in analysing spectroscopic titration data, *etc*. They will take full part in all group meetings and will present their progress in these meetings to the group as well as engaging in one-to-one meetings with several members of the team. As such, the student will get a well-rounded experience in research, in the preparation of data and in the presentation of their findings to experienced audience. Given the nature of the TG research group, a range of potential research projects will be offered (exact project title will be decided following discussion between supervisor and student). Some examples of the current work can be seen in the figure below as well through the recent references listed.

Figure: a) “Chiral Pd_2L_4 capsules from readily accessible Tröger’s base ligands inducing circular dichroism on fullerenes C_{60} and C_{70}”, *Angew. Chem. Int. Ed.* 2024, e202421137. DOI:10.1002/anie.202421137b) “Time-Resolved Fluorescence Imaging with Color-Changing, “Turn-On/Turn-On” AIE Nanoparticles”, *Chem*, 2024, **10**, 578-599. DOI: 10.1016/j.chempr.2023.10.001.c) “Lanthanide luminescent di-metallic triple-stranded helicates formed from bis-tridentate (1,2,3-triazol-4-yl)-picolinamide (tzpa) ligands and their higher order self-assemblies“, *Mat. Chem. Front*. 2025, **9**, 258-270. DOI: 10.1039/D4QM00816B

*We are not able to offer modelling/computational-type work for potential CMM students.

Prof. Andreas Heise & Dr. Viviane Chiaradia
RCSI

Discipline: Polymer Chemistry

Areas of Research (Keywords): Polypeptides, functional biomaterials, 3D printing, drug delivery, nanomaterials, renewable polymers

Summary of type of research projects that could be undertaken:
Our research focuses on the intersection of synthetic polymer chemistry and polymer processing to develop novel functional biomaterials. We design and synthesize polymers using techniques such as ring-opening and radical polymerisation, followed by comprehensive characterisation through NMR, FTIR, and chromatographic methods. A key aspect of our work is the precise control of polymer structures, including molecular weight, composition, and functional group positioning, to fine-tune material properties for specific applications. Beyond synthesis, we employ advanced processing techniques to shape these polymers into functional formats for applications in drug delivery, tissue engineering scaffolds, and, more recently, sustainable materials. This includes the fabrication of nanoparticles and the use of various 3D printing technologies to create tailored biomaterial architectures.

*Please clarify if you are able to offer molecular modelling/computational-type work for potential CMM students

Prof. Joanna McGouran

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Discipline: Organic Chemistry

Areas of Research (Keywords): Chemical Biology, Medicinal Chemistry, DNA damage repair, Bioresponsive materials, Peptide modification, Protein modification.

Summary of type of research projects that could be undertaken:

In the wake of 2022 Nobel Prize in Chemistry awarded to Carolyn Bertozzi, Barry Sharpless and Morten Meldal, the world has entered a golden era of chemical biology research. Our laboratory focuses on the synthesis and testing of molecules which can be activated in response to chemical or biological stimuli. Examples of Senior Sophister projects include:

Probing DNA damage repair.

These projects involve chemical synthesis and biological testing of inhibitors of the enzyme SNM1A. SNM1A is a key DNA damage repair enzyme. It plays vital roles in DNA repair, immune system development and telomere maintenance. Despite its clear biological importance in cancer therapy, immunity and ageing few inhibitors exist for SNM1A, or indeed any nucleases of this class. Inhibitors of SNM1A will be made by chemical synthesis of modified nucleotides, using methodologies recently developed in the laboratory.

Bio-responsive polymers.

The investigation of bio-responsive materials to date has been limited. Projects in this area will synthesise and test potential hydrogen peroxide responsive polymers, towards an ultimate goal of creating tumour responsive materials. Projects in this area can focus either on chemical synthesis of novel responsive monomers/crosslinkers or on the composition and response of polymeric materials using established monomers and crosslinkers.

Biologically active peptides.

We are in a new era for the discovery of peptide drugs, with over 33 non-insulin peptide drugs approved since 2000. These peptide drugs are no longer simply hormone mimics or composed simply of natural amino acids. These projects focus on the solid phase synthesis and subsequent modification of bioactive peptides to explore post-translational modification, peptide stapling, and pro-drug approaches.

Protein modification.

A project may be available in collaboration with Prof Derek Nolan (Biochemistry) studying bloodstream forms of African trypanosomes. These exclusively extracellular parasites survive and thrive in the mammalian vasculature and CNS. They have perfected strategies to evade the host antibody response, which we will model through protein modification.

More details for areas of our research and publications can be found on the lab website: https://joannamcgouran.wixsite.com/mysite. Please email me (jmcgoura@tcd.ie) if you would like to know more about any of the projects described.

*We are not able to offer modelling/computational-type work for potential CMM students.

Prof. Isabel Rozas

rozasi@tcd.ie

Supervisor Name: Isabel Rozas

Discipline: Organic, Medicinal & Biological Chemistry

Areas of Research (Keywords): Computational Medicinal Chemistry

Summary of type of research projects that could be undertaken:

We work in the design of guanidinium derivatives with potential as therapeutic agents.

Thus, we study the potential interactions of guanidinium diaryl derivatives with different targets of interest such as DNA or enzymes involved in tuberculosis or COVID19. In order to do that we optimise the ligands' structures by means of QM methods (in particular DFT or MP2) and then we use docking methodology (Autodock Vina) to see if they 'fit' into the active/binding sites of the aimed target. Additionally, we can theoretically assess different physicochemical and pharmacokinetic properties of the ligands proposed to see their suitability as potential drugs ("drugability").

*We **can** offer molecular modelling/computational-type work for potential CMM students

Prof. Eoin M. Scanlan

scanlane@tcd.ie

Discipline: Organic Chemistry

Areas of Research (Keywords): Medicinal Chemistry, Therapeutics, Antibiotics, Peptides, Carbohydrates, Methodology, Biomolecular Synthesis, Immunology,

Summary of type of research projects that could be undertaken: The Scanlan group has an active research programme in Synthetic Organic Chemistry with particular expertise in Thiol-ene chemistry, Peptide Synthesis and Glycoscience. Our aim is to design and synthesise novel biomolecules and bioconjugates including carbohydrate, lipid, peptide and protein conjugates as therapeutics. Our research is cross-disciplinary and involves collaboration with groups in Immunology, Biochemistry and Neuroscience. At the core of our research is the development of novel synthetic methodologies to access molecules of therapeutic interest.

Sample research projects include:

(i) **Synthesis and biological evaluation of novel analogues of Ozempic for treatment of type- 2 diabetes:** Receptor agonists of glucagon-like peptide 1 (GLP-1) are emerging as potent first-line treatments for the treatment of diabetes. In this project we will investigate novel chemical ligation methodologies to access and test new GLP-1 receptor agonists.[1]

(ii) **Synthesis and biological screening of novel anti-PD-L1 peptide inhibitors as checkpoint inhibitors for cancer immunotherapy:** Immunotherapy using checkpoint inhibitors, especially PD-1/PD-L1 inhibitors, has emerged as a promising therapy for cancer patients. The majority of these inhibitors are monoclonal antibodies, and their large size may limit tumor penetration, leading to suboptimal efficacy. As a result, there is growing interest in developing low-molecular-weight checkpoint inhibitors based on peptide scaffolds. In this project, we will develop and test novel peptide-based checkpoint inhibitors for applications in cancer immunotherapy (in collaboration with Prof. Ed Lavelle, TBSI)[2]

(iii**) Photocatalytic Thiol-ene Mediated Cyclisation Reactions:** In this project, the photocatalytic, intramolecular thiol-ene reaction will be explored for the chemical synthesis of small molecule ring systems as part of a natural product synthesis. Medium-sized heterocycles (9-membered rings) will be prepared by radical mediated methos and further modified towards natural product scaffolds for drug discovery.[3]

(Exact project title will be decided following discussion between supervisor and student)

*We are not able to offer modelling/computational-type work for potential CMM students.

(1). Scanlan E. M. *Nature Commun.* ***2017**, 8, 15655; Zheng. Z. Sig Transduct Target,* ***2024**, 9, 234.* (2). Scanlan, E. M. *Chem. Comm.* 2024, 60, 7950; Liu, C. *Cancer Cell Int* **2021**, 21, 239. (3) Scanlan* E. M. *J. Org. Chem.* **2023,** 88, 10020.

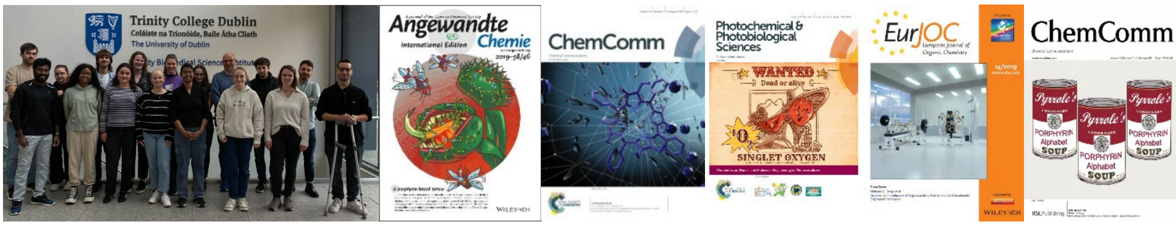
Prof. Dr. Mathias O. Senge

TBSI 6.28 / sengem@tcd.ie

Discipline: Organic, Medicinal and Biological Chemistry

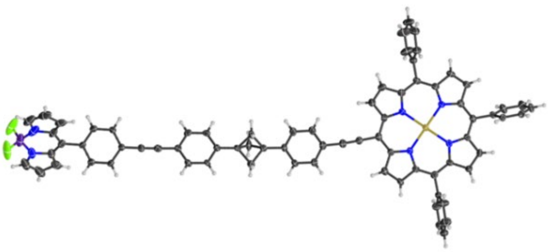
Areas of Research (Keywords):

Organic chemistry: synthetic organic chemistry; new synthetic methods; synthesis of hydrocarbon scaffold molecules, triptycenes, bicyclo[1.1.1]pentanes, cubanes; organometallic chemistry. Molecular engineering of topologically defined structures.
Biological chemistry: heterocyclic and natural product chemistry; porphyrins and tetrapyrroles; regulation of enzymatic reactions on a molecular level.
Medicinal chemistry: photomedicine, photodynamic therapy; theranostics, nanotherapeutics.
Photobiology: chlorophylls and photosynthesis; structure-function relationships in biological cofactors; photosynthesis.
Crystallography: structure determination and conformational analysis of natural products and coordination compounds; crystal engineering of tetrapyrroles, development of programs for database-driven conformational analysis.
Photochemistry: synthetic photocatalysis, stable peroxides, singlet oxygen reactions.
Material science: photonics materials; material isosteres; molecular circuitry, 2D nanostructures, on-surface chemistry and physics of functional nanomaterials.
History and philosophy of science: porphyrins, photochemistry and photomedicine.
ArtScience: Facilitating arts in science and science in arts.



Summary of type of research projects that could be undertaken:

Most projects will be in 'wet lab' synthetic organic chemistry and entail: methods development, reaction optimization, separation of reactions mixtures, and structural analysis. Requirements: Very good knowledge of mechanistic organic chemistry, spectroscopic analysis (NMR, UV/vis, MS) and chromatographic methods; ability to work under inert atmosphere.



The molecule on the left features most of the synthetic methods, tectons, and many of the applications we are currently interested in. If you know what they are and want to learn more …

(Exact project title will be decided following discussion between supervisor and student)

*We are not able to offer modelling/computational-type work for potential CMM students.

Senge Group

Prof. Mike Southern

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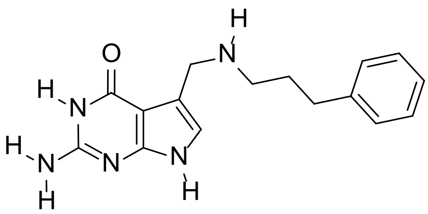
Discipline: Organic, Biological and Medicinal

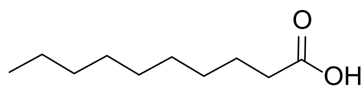
Areas of Research (Keywords): Synthetic chemistry, medicinal chemistry, autoimmune disease, epilepsy, addiction.

Summary of type of research projects that could be undertaken:

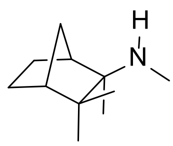
All projects revolve around the use of synthetic chemistry to make new compounds based on an ever-expanding knowledge of the key structural aspects required to influence the appropriate systems, in target diseases. Compounds successfully prepared will be tested by colleagues with the appropriate expertise.



NPPDAG



Decanoic acid



Mecamylamine

Autoimmune disease: This project is based on the development of derivatives of the little-known micro-nutrient queuine. Queuine cannot be biosynthesised by eukaryotes and must be obtained from the microbiome and/or diet. Queuine has been shown to influence the rate and fidelity of translation (protein synthesis) and we have shown that derivatives of queuine can influence the factors associated with autoimmune disease. This project will involve the synthesis of derivatives of the lead compound NPPDAG.

Epilepsy: The project is based on an idea to improve the active components of the ketogenic diet (high fat, very low carbohydrate) that has been shown to reduce the number and severity of epileptic seizures, particularly in children and patients who do not respond well to current treatments. Decanoic acid is a key metabolite in the diet that has been shown to influence glutamatergic signalling processes in the central nervous system. We are developing decanoic acid derivatives to provide improved biological activity and remove reliance on the unhealthy and unpleasant ketogenic diet.

Addiction: Mecamylamine is an old antihypertensive treatment that has been shown to have interesting anti-addictive properties. The compound exerts its biological effect by influencing nicotinic acetyl choline ion channels. We have shown that simple structural changes provides compounds that are more active and more selective than mecamylamine at important nicotinic acetylcholine receptor subtypes. The project will involve the further probing the effects of strategic structural changes.

*We are not able to offer modelling/computational-type work for potential CMM students.

Physical, Computational and Materials Chemistry Based Projects

Prof. Chris McAuley

McAuleyGroup.net Chris.McAuley@tcd.ie

Discipline: Physical Chemistry

Areas of Research (Keywords): Environmental Electrochemistry, Numerical Simulation, Energy Transformation, Electro-Organic Synthesis

Summary of type of research projects that could be undertaken:

Figure 1: Finite difference simulated diffusion limited reaction rate at a cubic nanoparticle. Yellow indicates areas of high interfacial flux.

Electrochemistry is at the heart of the green energy revolution. From batteries and solar cells to hydrogen production, interfacial electron transfer reactions are critical to many energy conversion technologies. While no single solution will resolve the global energy challenge, electrochemistry will undoubtedly play a key role in shaping a sustainable future.

In the **McAuley Group** (McAuleygroup.net), we take a **bottom-up approach** to understanding this essential class of reactions. Our research spans from fundamental studies on electron transfer and mass transport to nanoscale investigations of electrochemical processes. A core focus is on evaluating the efficiency and mechanism of electrocatalytic and interfacial reactions, ensuring that emerging technologies are both effective and scalable.

Research Areas

Beyond energy conversion, electrochemistry has far-reaching applications in analytical chemistry and synthetic methodologies. In collaboration with the Dunne Group, we develop and characterize novel metal oxide catalysts for electrocatalytic reactions. Additionally, we explore **low-cost sensor design** for analytical applications and investigate **electro-organic synthesis**. Electro-organic synthesis is a rapidly expanding field with significant potential for sustainable chemical manufacturing. Across these areas, our work is driven by a **rational design approach**, aiming to understand and control both homogeneous and heterogeneous reaction kinetics.

Opportunities for Students

We offer both **experimental** and **theoretical (computational) projects** (suitable for CMM and others), which complement each other in providing deeper insight into interfacial electrochemical processes. Our computational research relies on finite difference simulations, primarily implemented in Python, to model complex reaction dynamics. While coding experience is beneficial for theoretical projects, it is **not a requirement**, and support is available for those eager to learn.

If you are interested in working at the interface of theory and experiment to tackle pressing energy and chemical challenges, we encourage you to explore the exciting opportunities available in our group!

*We **can** offer modelling/computational-type work for potential CMM students.

Prof John Boland
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Summary of type of research projects that could be undertaken:

The are two possible areas for research projects:

The first type of projects will involve studies of the behaviour of metal films following annealing and recovery of nanocrystalline grains to assess the influence of grain growth and its impact on electrical properties. This may also involve an assessment of the evolution of the surface topography of the films, dewetting from the substrate, observed optically and by AFM.

The second type of projects involves studies of the behaviour of different plastics and the release of microplastics into water and the possible role of air bubbles at the plastic-water interface on this release phenomenon. Contact angles of air bubble will be measured on different substrates and their impact on the plastic substrate and the release of microplastic will be measured optically, by AFM and subsequent filtration.

*We are not able to offer modelling/computational-type work for potential CMM students.

Prof. Paula E. Colavita

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Discipline: Physical/Materials Chemistry

Areas of Research (Keywords):

Sustainable materials, sustainable coatings and thin films, circular economy technologies, electrocatalysis, energy conversion, carbon materials, transition metal oxides.

Summary of type of research projects that could be undertaken:
(Exact project title will be decided following discussion between supervisor and student)

Research in our group broadly seeks to develop tailor-made surfaces and surface modification processes to (a) achieve advanced functionality in a range of applications, and (b) to understand fundamental chemical processes that take place at interfaces. Research activities are at the intersection of materials, analytical and physical chemistry and there are opportunities for carrying out projects at the boundary with materials engineering, green chemistry and energy science.
Undergraduate experimental projects in the following areas might be available:

1. **Environmentally friendly surface treatments for improved metallization of polymers:** Effective metallization of plastics via electroless deposition and electroplating of metal thin films (e.g. Cu, Au etc) is an important step in the manufacturing of a wide range of devices. Pre-treatment protocols to ensure the adhesion and robustness of deposited metals are essential, however state-of-the-art pre-treatments involve aggressive etchants and hazardous chemicals that present safety and disposal concerns. Our team is working towards developing novel polymer surface pre-treatments that use mild conditions and environmentally safer chemicals to deliver metallized polymers with high metal-polymer adhesion, as shown via mechanical testing in Figure 1.[1] Chemical methods of surface engineering will be used by students in these projects to achieve high adhesion and validate performance. Students will acquire skills in the areas of surface modification, surface characterization and mechanical performance testing.

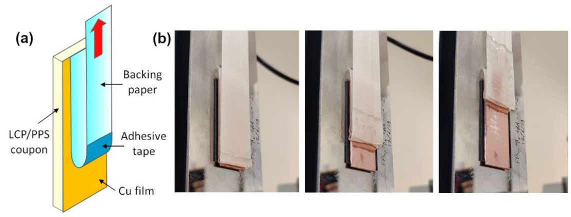

Fig.1: Measurements of adhesion strength of a copper thin film deposited on a polymer.[1]

2. **Sustainable materials for energy technologies:** Electrochemical energy technologies such as electrolysers, fuel cells and batteries are expected to play a key role in future energy solutions. However, state-of-the-art materials used for the above technologies are often based on the use of precious and/or scarce elements to electrocatalyse the electrochemical conversions of interest, thus posing problems of sustainability and cost. Our team is working towards developing and testing novel low-cost and sustainable electrode materials for the electrocatalysis of reactions that are important for electrochemical energy conversion. We take a two-pronged approach to this problem via design of model materials that enable a fundamental understanding of these processes, and via synthesis of nanostructured or surface engineered electrodes with potential for applications.

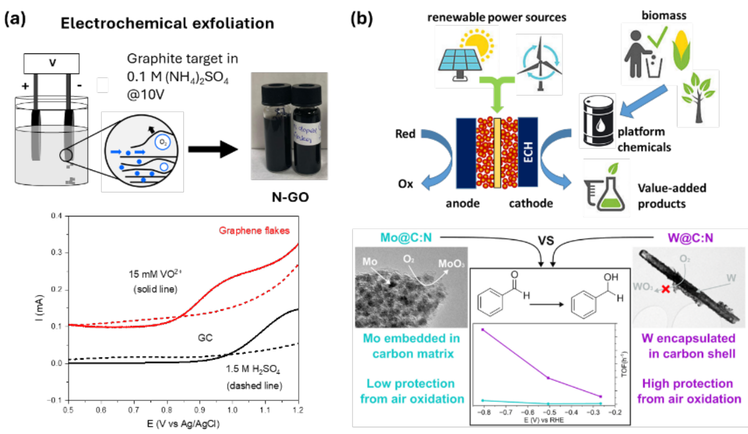

Fig.2: (a) Synthesis of graphene oxides (top) for electrocatalysis of V^{5+}/V^{4+} (bottom).[2,3] (b) Electrocatalytic hydrogenation for valorisation of organics (top) and M@C materials synthesized for hydrogenation of aldehydes to alcohols (bottom).[4]

3. Recent examples from the group are (Figure 2):[2-4] (i) development of carbon electrodes to understand performance in vanadium redox flow batteries; (ii) porous M@C heterostructured electrodes for electrochemical organic synthesis; and (iii) transition metal oxide electrodes for valorization of organics of biomass origin. Students undertaking projects in these topics will acquire skills in one or more of the following: electrochemical methods, materials synthesis/deposition, surface spectroscopy, product separations via chromatography (GC-FID, HPLC).

*We are not able to offer modelling/computational-type work for potential CMM students.

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1. Nolan, H.; Zen, F.; Gençer, A.; Henderson, L.; Kelly, M.; Pota, F.; Schröder, C.; Scanlan, E. M.; Colavita, P. E., Functional organic adlayers for controlling the adhesion strength of electrolessly deposited copper on super-engineering plastics. *Appl. Surf. Sci.* **2025,** *682*, 161700.
2. Costa de Oliveira, M. A.; Schröder, C.; Brunet Cabré, M.; Nolan, H.; Forner-Cuenca, A.; Perova, T. S.; McKelvey, K.; Colavita, P. E., Effects of N-functional groups on the electron transfer kinetics of VO^{2+}/VO_2^+ at carbon: Decoupling morphology from chemical effects using model systems. *Electrochim. Acta* **2024,** *475*, 143640.
3. Costa de Oliveira, M. A.; Brunet Cabré, M.; Schröder, C.; Nolan, H.; Pota, F.; Behan, J. A.; Barrière, F.; McKelvey, K.; Colavita, P. E., Single-Entity Electrochemistry of N-Doped Graphene Oxide Nanostructures for Improved Kinetics of Vanadyl Oxidation. *Small* **2024,** *n/a* (n/a), 2405220.
4. Pota, F.; Costa de Oliveira, M.; Schröder, C.; Brunet Cabré, M.; Nolan, H.; Rafferty, A.; Jeannin, O.; Camerel, F.; Behan, J.; Barrière, F.; Colavita, P. E., Porous N-doped carbon-encapsulated iron as a novel catalyst architecture for the electrocatalytic hydrogenation of benzaldehyde. *ChemSusChem* **2024,** *n/a* (n/a), e202400546.

Dr. Richard Hobbs

hobbsr@tcd.ie

Discipline: Physical Chemistry

Areas of Research (Keywords): Nanolithography, nanophotonics, nanomaterials, plasmonic materials, surface engineering, photodetectors and nanoscale light sources.

Summary of type of research projects that could be undertaken:

Atomic-scale defect control in hexagonal boron nitride for sustainable quantum light sources. Quantum technologies have long relied on devices that require cryogenic temperatures to maintain quantum properties. There is an urgent need to harness quantum effects beyond the cryogenic lab to achieve sustainable quantum devices. Conventional methods to produce single-photon sources for quantum devices focus on extending matter coherence times (slowing dephasing) at cryogenic temperatures. In this project, emitters are coupled to plasmonic cavities that support faster spontaneous emission rates to outpace dephasing at room temperature. The project will allow the student to gain experience of nanofabrication processes in a cleanroom environment, electromagnetic simulation of the interactions of plasmonic nanoparticles with light and characterization of plasmonic/2-d materials by electron microscopy and optical spectroscopy (see figures 1a,c,d,e).

Holographic matter-wave lithography. State-of-the-art lithographic processes used to produce integrated circuit patterns are based on extreme-ultraviolet lithography (EUVL) using photons having wavelengths of 13.5 nm (kinetic energy > 90 eV). Due to the large kinetic energy carried by EUV photons, electrons excited in the patterning medium (photoresist) can propagate several nanometers from the site of photon absorption leading to pattern blur. Matter-wave lithography using beams of metastable helium atoms provides a route to reduce this blur, by reducing the amount of energy transferred to electrons in the resist layer. The project will allow the student to gain experience of nanofabrication processes in a cleanroom environment, electron microscopy of nanomaterials, etch chemistry and fabrication processes used to produce matter-wave optics (see figure 1b).

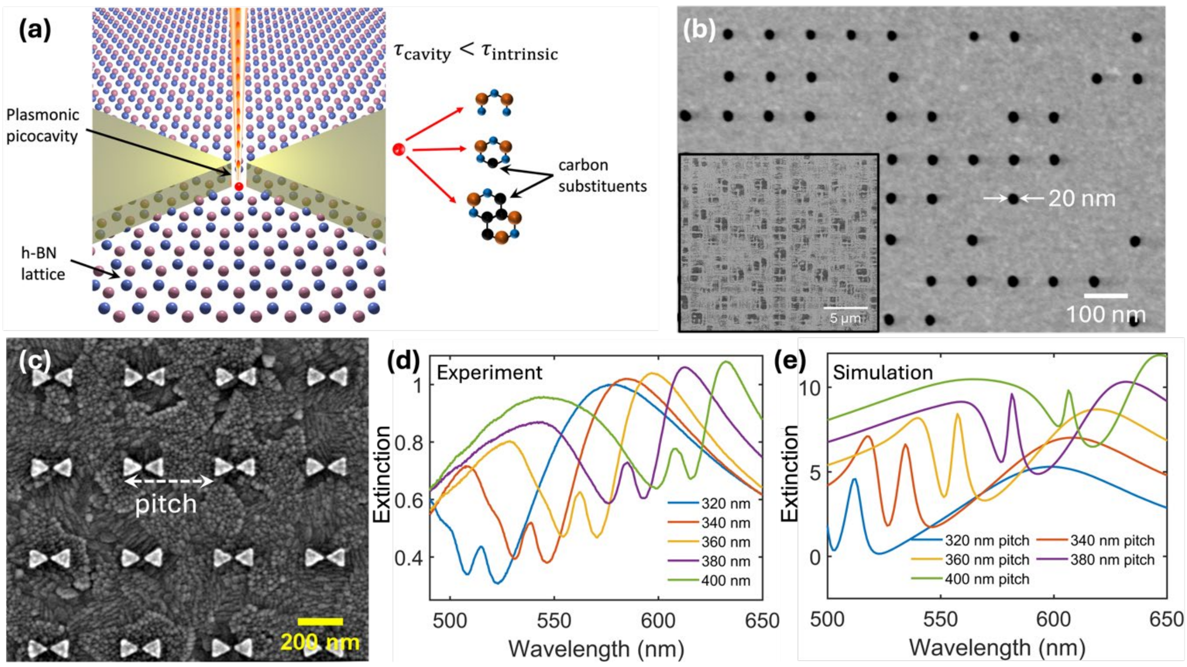


Figure 1. *(a) Atomic-scale defects in 2-d materials such as h-BN can be exploited for the development of single-photon sources. Controlled placement of defects (vacancies/substitutions) within nanoscale plasmonic cavities can be used to develop sources with characteristics suited to devices for quantum technologies. (b) Scanning transmission electron microscope (STEM) images of arrays of nanopores in 10-nm-thick SiN_x membranes (inset, low-magnification STEM image of hologram). (c-e) Arrays of plasmonic Al bow-tie nanoantennas exhibiting pitch-dependent spectral resonances.*

*We are not able to offer modelling/computational-type work for potential CMM students.

Prof. Tobias Kraemer

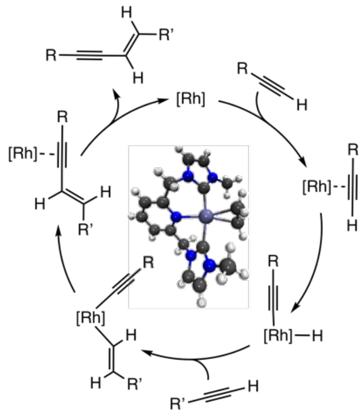
KRAEMERT@tcd.ie

Discipline: Computational Chemistry, Inorganic Chemistry

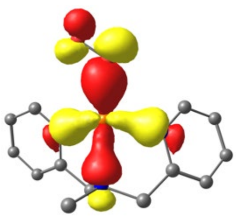
Areas of Research (Keywords): Catalysis, Organometallic Chemistry, Main Group Chemistry, Coordination Chemistry, Electronic Structure, Theoretical Spectroscopy, Small Molecule Activation

Summary of type of research projects that could be undertaken:

(Exact project title will be decided following discussion between supervisor and student)



Project Area 1: Theoretical Catalysis The catalytic transformation of chemical bonds to produce new chemicals and materials of intrinsic value to society is a key focal point of current chemical research. We model multi-step catalytic cycles to get insight into the mechanistic details of these reactions at the electronic structure level, ultimately with the goal in mind to guide the rational design of improved catalyst platforms. Systems that we study include complexes of both base (Fe, Co, Ni) and precious (Rh, Ir, Pd, Pt), as well as main group (Al, Ga, Ge) metals with a large variety of ligand architectures that are utilized in both homogenous and heterogeneous catalysis. You will be able to explore the electronic structure of a choice of catalysts containing Rh, Ti, Ga or Al centres. The main objective will be to map out the energetic landscape of their chemical reactions using quantum chemical calculations. Key publications: K. M. Byrne, J. Hicks, L. P. Griffin, S. Aldridge, T. Krämer, *Chem. Eur. J.*, **2025**, *31*, e202500095; K. M. Byrne, S. D. Robertson, R. E. Mulvey, T. Krämer, *ChemCatChem*, **2024**, *16*, e202400655. M. R. Gyton, I. Bustos, M. J. G. Sinclair, S.-y. Tan, C. J. Wedge, S. A. Macgregor, A. B. Chaplin, *J. Am. Chem. Soc.*, **2023**, *145*, 14087. R. Falconer, K. M. Byrne, G. S. Nichol, T. Krämer, M. J. Cowley, *Angew. Chem. Int. Ed*., **2021**, *6*, 24702.



Project Area 2: Bioinorganic Chemistry Understanding the fundamental catalytic processes facilitated by enzymes remains a major challenge in energy research. Enzyme systems utilize earth-abundant base metals in their active sites yet can affect the activation of inert chemical bonds very efficiently. Our objective is to provide insight into the electronic structures of the active sites and their chemical transformations at the atomic structure level. Critically interlinked with this aspect are low-weight molecular complex systems that aim to mimic the structural and functional behaviour of native enzymes. We combine computational methods with theoretical spectroscopy to gain information about the oxidation states, spin states, and the local coordination environments of the transition metal active sites. Specifically you will study the propensity of a four-coordinate superoxo cooper (II) complex in hydrogen atom transfer (HAT) from various organic substrates.
Key publications: S. Debnath, S. Laxmi, O. McCubbin Stepanic, S. Y. Quek, M. van Gastel, S. DeBeer, T. Krämer, J. England, *J. Am. Chem. Soc.*, **2024**, *146*, 23704; S. Y. Quek, S. Debnath, S. Laxmi, M. van Gastel, T. Krämer, J. England, *J. Am. Chem. Soc.*, **2021**, *143*, 19731.

During a project in the Kraemer group, students will gain experience in operating on UNIX platforms, setting up molecular models, perform atomic-scale quantum chemical simulations with a variety of software packages, and analyse and interpret data generated by these programs.

*We **can** offer modelling/computational-type work for potential CMM students.

Prof. Mike Lyons

melyons@tcd.ie

Supervisor Name: Professor Mike Lyons

Discipline: Physical, Materials and Computational Chemistry

Areas of Research (Keywords): Physical and materials electrochemistry

Summary of type of research projects that could be undertaken:

Research in the Lyons Group has a focus on examining the growth mechanism, redox and capacitive behaviour and electro-catalytic properties of metal oxy-hydroxide thin films grown via electrochemical means on Fe, Ni, Co or Mn electrodes in aqueous alkaline solution. These hydrated oxy-hydroxide thin films have demonstrated excellent potential for the catalysis of water oxidation, the oxidation of organic alcohols and biomolecules, and the reduction of molecular oxygen to form water. These materials also exhibit excellent charge storage and pseudo-capacitive behaviour.

*We **can** offer molecular modelling/computational-type work for potential CMM students

Prof. Valeria Nicolosi
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Discipline: Physical Chemistry

Areas of Research (Keywords):
Nanomaterials synthesis and processing, energy storage, batteries, supercapacitors

Summary of type of research projects that could be undertaken:

Synthesis, Characterisation, and Application of 2D Nanomaterials for Energy Storage Devices

SS Capstone projects in the Nicolosi group will offer an exciting and multifaceted opportunity for students to explore the synthesis, processing, or the characterisation of 2D nanomaterials, or to focus on their application in energy storage systems such as batteries and supercapacitors. Under the guidance of Prof. Nicolosi, students will have the flexibility to tailor the project to their main interests, allowing them to dive deep into the areas of synthesis, materials science, characterisation or energy storage technologies. Students will have the opportunity to choose a specific area of interest within the project scope, whether focusing on the synthesis of new materials, the development of advanced processing techniques, or the design and testing of energy storage devices.

Synthesis of 2D Nanomaterials:

- Students will learn and apply solid-state reaction techniques to synthesise a variety of 2D nanomaterials, such as MXenes (Transition metal carbides and carbonitrides).

Processing in Liquid Phase:

- Students will explore methods for processing 2D nanomaterials in the liquid phase to optimise dispersion, stability, and integration into energy storage devices.
- Techniques such as ultrasonication processing and sol-gel methods will be employed to prepare nanomaterial dispersions suitable for use in batteries and supercapacitors.

Characterisation of Nanomaterials:

- A crucial part of the project will involve characterising the 2D nanomaterials to understand their structural, chemical, and electronic properties.
- Students will gain experience with advanced characterisation techniques such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), Raman spectroscopy, and electrochemical testing.

Energy Storage Applications:

- Students will study the potential of synthesised and processed 2D nanomaterials in energy storage applications, with a particular focus on batteries and supercapacitors.
- Performance testing will include the fabrication of electrodes and the evaluation of key metrics such as charge/discharge cycles, specific capacitance, energy density, and power density.

*We are not able to offer modelling/computational-type work for potential CMM students.

Prof. Graeme Watson

watsong@tcd.ie

Supervisor Name: Graeme Watson

Discipline: Physical, Computational and Materials Chemistry

Areas of Research (Keywords): Computational Materials Chemistry, Density Functional Theory, Molecular dynamics, Energy Materials, Catalysis

Summary of Research Projects that could be undertaken: Materials modelling is a cutting-edge field that leverages computational techniques to predict and understand the properties and behaviour of materials at the atomic and molecular levels. Our project aims to use advanced techniques to simulate the structural, electronic, ionic, electrical conductivity, and mechanical properties of novel materials. By utilizing state-of-the-art software and high-performance computing resources, we explore the potential of these materials for various applications, including energy storage and generation, electronic materials, and catalysis. Techniques are selected based on the materials and properties desired and include Classical molecular dynamics, Density functional theory and Machine learning forcefields. The insights gained will not only enhance our fundamental understanding of material science but can pave the way for innovative solutions to real-world challenges.

Energy Materials: Current projects within the group focus on energy materials, including fluoride ion batteries (FIBs) and solid oxide fuel cells. The development of these requires solid-state materials with improved fast ion conduction. A combination of database searching, screening, and modelling can be used to search for new materials with improved properties. Defects play a critical role in the diffusion properties, including the impact of grain boundaries in multi-crystalline materials, which can have a negative or positive impact on diffusion (figure 1).

Catalysts Development: Other areas include the development and understanding of new catalysts, such as those for CO_2 conversion. This research can use a variety of metals (including alloys) or doped oxide catalysts, with modelling used to understand the impact of the local reaction centre on the reaction pathway and activation energy.

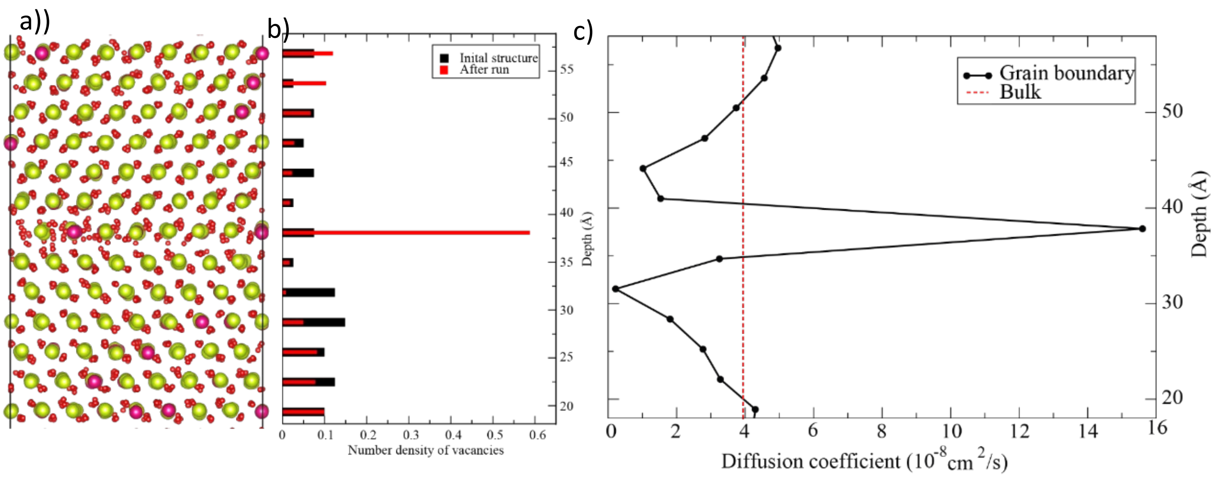

Figure 1 Results from a MD simulation of the $\Sigma3(111)$ GB of $Ce_{0.9}Sm_{0.1}O_{1.95}$. a) Structural model, b) oxygen vacancy distribution before and after annealing and c) resulting ionic diffusion parallel to the interface.

*We **can** offer modelling/computational-type work for potential CMM students.