

MSc Chemical Research Potential Supervisors 2019/20

1. Isaac Abrahams

My Research interests are in solid state chemistry. I am happy to offer projects in the following areas:

1. New systems as glass ionomer cements for surgical applications
2. Anti-cancer drug delivery using calcium phosphate nanoparticles
3. Local ordering in solid electrolytes using reverse Monte Carlo modelling of total neutron scattering

I am happy to offer other projects depending on the student's interest.

2. Stelios Arseniyadis

The group is principally interested in the discovery, development and study of new synthetic methods to attain high structural and functional complexity. These methods mainly span within the areas of transition metal catalysis, and, more recently, bio-inspired asymmetric catalysis. At the core of our research is the will to provide innovative, efficient but also multivalent tools for natural product synthesis and drug discovery.

For more information: https://arseniyadislab.sbcs.qmul.ac.uk/?page_id=681

Publication page: https://arseniyadislab.sbcs.qmul.ac.uk/?page_id=680

3. Christopher Bray

Please see <http://www.sbcs.qmul.ac.uk/staff/christopherbray.html> for more details.

4. Xacobe Cambeiro

Please see <http://www.sbcs.qmul.ac.uk/staff/xacobecambeiro.html> for more details.

5. Gregory Chass

Please see <http://www.sbcs.qmul.ac.uk/staff/gregorychass.html> for more details.

6. Rachel Crespo-Otero

In our group, we work on the application and development of methods to understand the interaction of light with matter. We are particularly interested in phenomena at the interface between molecular and material sciences.

Our main research lines are

- Excited states and dynamics simulations
- Modelling of chemical reactions in the ground and excited states
- Modelling of excited state processes in the crystal environment

7. Devis Di Tommaso

The research group of Dr. Devis Di Tommaso focuses on the development and application of computational chemistry techniques to solve a wide range of problems in Physical and Materials Chemistry.

We are particularly interested in modelling processes of crystal nucleation and growth of organic and inorganic materials from complex solutions. Our aim is to understand how the chemistry of solution (nature of the solvent and type and concentration of solution additive) controls the kinetics of crystal growth and the process of polymorph selection during crystallization from solution.

A new research departure venture in our group is also the development of atomistic simulation methods (mostly quantum mechanical ones but also Monte Carlo and molecular dynamics) for the design of nanocatalysts for the efficient and selective transformation of CO₂ into value-added chemicals. We employ a variety of theoretical techniques including electronic structure methods, first principles and classical dynamics, and continuum approaches and we make extensive use of supercomputing facilities.

Group webpage: webspaces.qmul.ac.uk/dditommaso/index.html

8. Arianna Fornili

The research activity of the group is focused on the computational study of protein dynamics and its relationship to protein function.

The main interest of the group is the study of structural, dynamical and mechanical properties of proteins from the cardiac muscle. Heart contraction arises from a complex interplay of precisely timed molecular motions and the identification of new therapeutic targets for cardiomyopathies relies on a deep understanding of these mechanisms. Combining Molecular Modelling, Molecular Dynamics simulation and Bioinformatics techniques, we investigate the protein motions under normal and pathogenic conditions and we use this information to develop new drugs.

The group is also involved in the development of computational methods for the study of conformational transitions in proteins. In addition to promoting the motion of molecular motors, conformational changes can be essential for many protein functions and they are often required for protein-protein interaction and allosteric regulation. The group aims at improving both the sampling and the detection of biologically relevant conformational transitions, which are usually beyond the timescale of traditional molecular simulations.

Techniques: Molecular Dynamics simulations, Homology Modelling, Molecular Docking, virtual screening, data analysis with R.

9. Cristina Giordano

Research in the Nanostructures Design and Shaping Group

Research aims: Expanding the knowledge on Nano Metallic Ceramics both for fundamental and applied science. Making them complementary/alternative to metal oxides and pure metals on a large scale.

Research in our group focuses on the design of novel/tailored pathways for the synthesis of advanced nanostructures based on metals, metal alloys and metallic ceramics (namely transition metal nitrides and carbides).

Metallic ceramics in particular possess a combination of properties that place them between classical ceramics and pure metals.

Most recently, our research also focuses on multifunctional materials, colloidal dispersions and hybrids based on MN/MC nanoparticles.

In particular, on the design of tailored multifunctional materials (hybrids and nanocomposites) based on metallic ceramics, where solid state bridges soft matter to create unique materials for target applications (e.g. catalysis, including photo- and electro-catalysis, batteries, supercapacitors, and more).

10. Lesley Howell

Research in our group is focused on protein-protein interactions (PPIs) and harnessing their potential as drug targets. We do this by using both solution and solid phase synthesis to generate compounds/peptides capable on interacting with these targets. We take inspiration from natural products when designing compounds but also design new molecules from scratch. Within this theme we have several projects:

Reactivation of the Bcl-2 mediated apoptosis pathway as a way to treat cancer

Development of new approaches/technology to target PPIs

Disruption of G-protein coupled receptor (GPCR) heteromers as novel drug targets

Identification and synthesis of ligands for orphan GPCRs

11. Christopher R Jones

We are interested in developing new synthetic organic methodology that has the potential to impact upon contemporary socioeconomic issues such as new drug discovery and the need to find more sustainable chemical feedstocks. As such, we aim to harness the high levels of reactivity of arynes, carbenes and radicals (“reactive intermediates”), as they afford unique and powerful opportunities to control challenging new chemical and biological processes. In our group we are particularly focused on exploiting aryne reactivity for the development of new synthetic strategies, including direct C(sp³)-C(sp²) bond formation and aliphatic C-H bond functionalisation, that will enable cheap and abundant hydrocarbon sources to be utilised and therefore reduce our reliance upon more limited and heavily functionalised starting materials

Link: <https://joneschemistry.wordpress.com>

12. Christian Nielsen

Work in our group (<https://nielsen-lab.com/>) is inspired by the Nobel Prize winning discovery of organic polymers that can conduct electricity. Such conducting polymers have been used extensively for example in organic light-emitting diodes and organic solar cells. In the Nielsen Lab, we are particularly interested in using conducting molecules and polymers in new fields including 1) organic bioelectronics, where these materials interface with biological systems for example by means of stimulation or sensing and 2) organic thermoelectrics, where the materials are utilised to convert waste heat, for instance from vehicles and factories, to electricity.

Most of our day-to-day work in the lab is centred around the synthesis and characterisation of new aromatic molecules and polymers. Projects in the Nielsen Lab will thus provide excellent training in standard organic chemistry laboratory techniques as well as characterisation techniques such as NMR and UV-Vis spectroscopy, cyclic voltammetry (CV) and X-ray diffraction (XRD). Comparing the synthesised materials and their key properties will allow for important structure-property relationships to be derived. With research collaborators, these new materials will subsequently be tested in conventional organic electronic devices such as field-effect transistors and in novel prototype bioelectronic or thermoelectric devices. This will provide highly valuable experience in multi-disciplinary research collaborations. Master's students will work closely with senior PhD or postdoc researchers in the group.

13. Matteo Palma

We are a physical chemistry group focusing on the controlled assembly of functional nanostructures, with single-molecule resolution. In particular, we are interested in using (supra)molecular interactions to drive the self-organization of nano-moieties from solution to nanopatterned substrates. We typically employ two different building

blocks for this: carbon nanostructures (as nano-electrodes) and DNA origami (as nanoscale scaffolds). Applications range from studies in the field of molecular (opto)electronics, to biosensing and biological investigations at the single-molecule level.

Please see <http://webpace.qmul.ac.uk/mpalma> for further information on current research and for recent publications.

14. Marina Resmini

Please see <http://resminilab.sbcs.qmul.ac.uk/> for more details.

15. Maxie Roessler

Oxidation-reduction (redox) reactions underpin innumerable chemical reactions - and much of the chemistry of life! We investigate how oxidation-state changes govern respiration and photosynthesis and how nature has fine-tuned the redox properties of its many intricate molecular machines. Redox reactions often involve transition metal ions and we are unravelling the properties, structure and bonding of transition-metal centres in both biological and synthetic molecular machines.

Many redox reactions proceed via radical intermediates and these are, perhaps luckily, often located in mechanistically key locations. In the lab, we use electron paramagnetic resonance (EPR) spectroscopy as a powerful method for obtaining detailed information on the structure and bonding these ubiquitous spin centres. Electrochemistry on the other hand, in particular film electrochemistry, provides insight into the reactions carried out by molecular machines. These (bio)physical methods are supplemented by biochemical and synthetic methods.

Please see <http://webpace.qmul.ac.uk/mroessler/> for further information on current research and for recent publications.

16. Tippu S. Sheriff

Catalysis, coordination and green chemistries: Activation of dioxygen and in situ hydrogen peroxide generation under ambient conditions for bleaching, selective oxidation; corrosion control and disinfection

The modelling of small molecule activation in biological systems such as catechol oxidase, with current interests in the catalytic activation of dioxygen and the in situ generation of hydrogen peroxide. Applications include low temperature bleaching, selective oxidation, corrosion control and disinfection and the generation of labelled hydrogen peroxide species (e.g. D₂¹⁸O₂). These interests involve the synthesis and characterization of novel manganese complexes and prototypes for the detection of hydrogen peroxide vapours, dioxygen and manganese.

Please see <http://www.researchpublications.qmul.ac.uk/publications/staff/20083.html> for recent publications.

17. Tony Vlcek

Transition metal chemistry, photoinduced electron transfer and charge separation, photophysics and photochemistry, photocatalysis, solar energy conversion by chemical means.

<http://www.sbcs.qmul.ac.uk/staff/tonyvlcek.html>

18. Peter Wyatt

I am a synthetic organic chemist with an interest in making substances of relevance to both life sciences and materials science. I work particularly with organic molecules containing the elements nitrogen, phosphorus and fluorine, as well as complexes of such ligands with d and f block metal ions.

I collaborate with groups working in these areas at Queen Mary and internationally. We have made and patented highly fluorinated, light emitting compounds for use in amplifying the optical signals that form the basis of global telecommunications and have recently set up the spin-out company Chromosol to develop these results further. I also provide the organic chemistry expertise within an international consortium to identify and study environmental toxins derived from the rare amino acid beta-N-methyl-L-alanine (BMAA), produced by cyanobacteria that are widespread in aquatic.

Please see <http://www.researchpublications.qmul.ac.uk/publications/staff/19519.html> for recent publications.

19. Ali Zarbakhsh

My research has always had a very strong inter-disciplinary and applied character with a focus on providing structure-function relationships for self-assembling surfactants and polymeric materials at interfaces. The major contributions have been in the development of experimental scattering techniques to resolve molecular structures at the buried fluid-fluid interface. This is now seen as critically important by those who are interested in catalysis, emulsions, electrochemistry, transfer, soft matter mixtures and biophysics at liquid-liquid interfaces. Current area of interest is a model for lipid emulsion drug delivery systems and interaction of a lipid monolayer with negatively charged polyelectrolytes.

My recent research has been in the area of (i) thermal responsive nanogels, resolving their conformations and their interactions with lipids mono and multilayers for drug delivery (ii) Developing a new class of biosensor for water quality testing (iii) the structural study of polymers and surfactants at the buried oil-water interface (iv) alkylated graphene multilayer structure deposited on solid support for self-assembly.

The other area of my research is adsorption on solid surfaces that can modify their properties and reactivity such as those associated with hydrophobicity, surface charge and others which govern interfacial processes, in particular, the study of tribological molecular systems to probe the molecular behaviour of oil additives under realistic conditions of shear and temperature.