

# NTU DOCTORAL SCHOOL

NOTTINGHAM TRENT UNIVERSITY 

*"Creating future innovators and impact for education, industry,  
the professions and society"*

Nottingham Trent University  
**Doctoral School**  
School of Science and Technology  
PhD Projects – 2016

Broad area of research – Chemistry and Forensic Sciences

# **Welcome to the Nottingham Trent University Doctoral School**

The Doctoral School provides a supportive environment and a thriving research culture that encourages you to reach your full potential as a research degree student.

## **Valuing ideas, enriching society**

We encourage new ideas and new ways of thinking across the whole University through a culture of discovery and innovation. We believe our research has the potential to impact the world we live in and change lives.

## **Research excellence**

Our research is recognised across the world. In the most recent Research Excellence Framework (Ref 2014) most of our research was considered internationally-excellent or world-leading.

The University is committed to developing and expanding its activity to increase the scope, quality and impact of our research.

## **Be part of our research**

With MPhil, PhD and Professional Doctorate research degree opportunities across each of our academic schools, we support students conducting research in a diverse range of areas. Our research students form an important part of our research community and make a significant contribution to our activity.

We offer full-time, part-time and distance learning research degree opportunities.

Our Professional Doctorates offer you the opportunity to contribute to research in your profession while attaining a research qualification.

## **A supportive community**

We are committed to supporting and developing our research students.

You will have academic, administrative and personal support throughout your studies and access to dedicated workspace and exceptional facilities.

## **Excellent support throughout your studies**

The Doctoral School aims to provide excellent personal and practical assistance for our research students creating a supportive and pro-active environment.

### **Support and guidance**

Your main source of advice and support will be your own doctoral supervisory team, which will include a director of studies and at least one other supervisor. This team will be selected based on their experience in your chosen area of study or their background in relevant practice.

The Doctoral School Team will be available throughout your studies. Our dedicated team will offer advice and guidance for your initial enquiry and application and introduce you to the University and to your supervisory team.

### **Outstanding facilities**

As a research student at NTU you will have access to a wealth of facilities and resources to aid and enhance your studies. The University is committed to providing the best possible facilities for all its students and we are constantly investing in new facilities and learning environments.

### **Dedicated study areas**

All our research students are able to use study and writing areas giving you access to desks, laboratories and IT facilities when you need it.

### **Learning resources**

Students at Nottingham Trent University have access to a wealth of library materials including over 480,000 books and 1,300 printed journals, as well as an extensive audio-visual collection of DVDs, videos and slides.

Electronic library resources are an increasingly important part of the support offered to research students, and more than 290 databases and 17,000 eJournals are accessible from any networked PC within NTU, or from your home or off-campus PC.

Our experienced and knowledgeable library staff will help guide you to the most useful sources of information.

## **Developing the next generation of researchers**

We aim to nurture research talent and help our students thrive through their research degrees and into their future careers.

### **Researcher Development Programme**

All research students are expected to participate in a rolling programme of professional development. You will have the opportunity to attend a range of workshops and developmental activities mapped to the Vitae Researcher Development Framework (RDF).

Our Research Development Programme empowers you – in discussion with your supervisory team – to create an individualized package of activities to support your career development as a researcher.

A range of core activities will support your journey from enrolment at NTU as a research student, through to final submission of your thesis. These activities will be complemented by a series of electives that you will choose to pursue, depending upon your developmental needs as you progress in your research work.

### **Developing your career**

We pride ourselves on equipping our students with knowledge and skills and encouraging initiative, innovation and excellence.

Our research students are encouraged to take part in conferences, seminars and external networks. These are an excellent opportunity for you to share your work, meet other researchers and build a network of contacts.

Our own research conferences and seminars offer you the opportunity to present and discuss your work among the NTU research community.

You may also have the opportunity to teach undergraduate students or supervise laboratory work.

# School of Science and Technology

Research in the School of Science and Technology is rich and diverse, with staff conducting internationally recognised and world-leading research. Research is clustered in Research Centres and units, providing a focus for different themes with their underpinning platforms:

- **Biomedical Sciences and the John Van Geest Cancer Research Centre**

Internationally excellent research environment – Our Biomedical Research is world-leading and involves staff with broad academic backgrounds, including Biochemistry, Bioinformatics and Biomathematics, Analytical/Synthetic Medicinal Chemistry, Immunology, Microbiology and Pharmacology. In the recent REF2014 assessment (<http://www.ref.ac.uk/>) of University research quality the Biomedical Sciences Research Unit's submission (to UoA A03) was highly rated, having 86% of overall activity at the highest 3\* (internationally excellent) and 4\* (world-leading) grades. This included achieving 100% of its impact at 3\* and 4\* levels.

- **Materials and Engineering**

Internationally excellent research environment – Our multidisciplinary Materials and Engineering Research is extremely strong in terms of high quality outputs, income generation, and international impact. In the recent REF2014 assessment of University research quality our Materials and Engineering Unit's submission (to UoA B15) was highly rated, having 84% of overall activity at the highest 3\* (internationally excellent) and 4\* (world-leading) grades. This included achieving a joint 7th rank out of 62 submitted UK institutions for the quality of our publications, which were judged as attaining 94.6% at 3\* and 4\* levels.

- **Computing and Informatics**

Internationally excellent research impact- The multi-disciplinary research is directed to address important questions and is clustered under three themes: [Interactive Systems](#) for cognitive and physical rehabilitation and mental wellbeing; [Computational Intelligence and Applications](#) for computationally intelligent methods and techniques; and [Intelligent simulation, modelling and networking](#). In the recent REF2014 assessment of University research quality the Computing and Informatics Research Unit's submission (to UoA B11) was highly rated achieving 80% of its impact at 4\* and 3\* levels.

- **Sport, Health and Performance Enhancement (SHAPE) Research Centre**

Internationally excellent research outputs- In the recent REF2014 assessment (<http://www.ref.ac.uk/>) of University research quality the Sport Sciences Research Unit's submission (to UoA C26) was highly rated, having 94% of the outputs rated at the 3\* (internationally excellent) and 2\* (internationally recognised) grades. Our Sports Science research is multi-disciplinary and is clustered under a number of themes, driven by the Musculoskeletal Physiology, Sports Performance, Exercise and Health and Sport in Society Research Groups.

## Research themes and areas

These research units promote the research excellence and facilities within the School, and stimulate knowledge transfer, innovation and exploitation. They provide strategic direction in research planning and portfolio development, and ensure that mechanisms are in place to nurture research.

List of available projects and a summary description of them are provided in the following research categories.

- [Biomedical Sciences and the John Van Geest Cancer Research Centre](#)
- [Computing and Informatics](#)
- [Materials and Engineering](#)
- [Sport, Health and Performance Enhancement Research Centre](#)

Or they can be searched based on the following academic Departments.

- [Biomedical and Biological Sciences](#)
- [Chemistry and Forensic Sciences](#)
- [Computing and Technology](#)
- [Physics and Mathematics, and](#)
- [Sport Science](#)

## **Project Titles (descriptions below)**

1. Prof. Steve Allin - Neighbouring Group Direction in Asymmetric Glycosylation
2. Prof. Steve Allin - Novel drug-dendrimer conjugates as novel treatments for ovarian cancer
3. Dr. Michael Coffey - Assessing indicators and management conditions for predicting polyphenol contents in wine production
4. Dr. Warren Cross - C-H functionalization for the diverse post-synthetic modification of peptides and proteins
5. Dr. Warren Cross - C(sp<sup>3</sup>)-H activation without a directing group
6. Dr. Warren Cross - Computational modelling of biomolecule C-H functionalization reactions
7. Dr. Muriel Funck - New tools for detection of biological and forensic evidences
8. Dr. Fengge Gao - Antimicrobial nano-hydrogel with healing functions
9. Dr. Fengge Gao - Nano-structured dielectric materials for energy application using gel coating nanotechnology
10. Dr. Fengge Gao - Novel stain-free materials with ability to absorb moisture
11. Dr. Fengge Gao - Ultra-light thermal and oxidation resistant materials
12. Dr. Chris Garner - Dipeptides for Treating Diabetes
13. Dr. Chris Garner - Kinetic Resolution Strategies for Chiral Secondary Phosphine Oxides
14. Dr. Quentin Hanley - The Analysis of Large Clusters by Fluorescence Anisotropy
15. Dr. John Hearn - Water Based Coatings for Pharmaceutical Dosage Forms
16. Dr. John Hearn - Composite Thin Polymer Latex Films

17. Dr. David Kilgour - Developing a high confidence multiplexed assay for protein toxins for food security
18. Dr. David Kilgour - A new, novel liquid interface for mass spectrometry
19. Prof. Carole Perry - New approaches to studying biomolecule-material interactions
20. Dr. Valeria Puddu - TiO<sub>2</sub> based hetero-structures for solar light technologies
21. Dr. Valeria Puddu - TiO<sub>2</sub> structures for solar light technologies.
22. Dr. Valeria Puddu - TiO<sub>2</sub> nanomaterials for electrochemical sensing.
23. Dr. Nitin Seetohul - Legal Highs are they legal?
24. Dr. Emma Smith - Materials Chemistry: The Deposition of Antimony from Deep Eutectic Solvents (DESS)
25. Dr. Emma Smith - The design of new electrochemical sensors
26. Prof. John Wallis - Synthesis of Libraries for Biological Testing Based on Novel Heterocyclic Chemistry
27. Prof. John Wallis - Organic Chemistry: Synthesis and Structural Investigation of Molecules with Partial Bond Formation
28. Dr. Warren Cross - C-H activation methods for the functionalization of bipyridines



# 1.

## NEIGHBOURING GROUP DIRECTION IN ASYMMETRIC GLYCOSYLATION

Glycoconjugates form a group of products that are among the most structurally diverse and densely functionalised in nature. Moreover they play essential roles in a multitude of biomolecular processes in areas as varied as neuronal development through to tumour growth and metastasis. The synthesis and study of complex carbohydrates has therefore become, and continues to be, an area of active research.

Historically, approaches to stereocontrol in glycosidation chemistry have included solvent effects, neighbouring group participation and anomeric equilibration. More recent contributions to this area have included Boons' novel refinement of the neighbouring-group participation approach to stereocontrolled glycosylation, using thioethers to deliver □selectivity as a complement to the more established use of C-2 esters. Disposable tethers and palladium catalysis have also been used to effect □limited activity in range of substrates and Fairbanks has also made a significant contribution in his study of chiral Bronsted acids to induce a diastereoselective coupling. Disappointingly these recent efforts have met with limited success and although neighbouring group participation is effective for controlling the '1,2 trans' geometry in glycosylation there is still no universal strategy for delivering the 1,2 cis arrangement.

**Supervisors:** Prof. Steve Allin

### Supervisor biogs

Professor Steven M. Allin is a graduate of Liverpool University, obtaining both a BSc in 1990 and, in 1993, his PhD under the supervision of Prof. Philip Page. Dr. Allin then studied as a postdoctoral research associate at the University of Florida with Professor Alan Katritzky before returning to the UK as a Lecturer at the University of Huddersfield. In January 1997 he moved to Loughborough University, was promoted to Reader in 2005 and in 2008 he moved to Keele University as Professor. Professor Allin has supervised 30 Ph.D. students and 11 postdoctoral researchers leading to over 75 publications. His research group has previously received support from EPSRC, the Leverhulme Trust and considerable support from the pharmaceutical and agrochemicals sectors.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry, Biochemistry or related discipline**.

Contact details: [steve.allin@ntu.ac.uk](mailto:steve.allin@ntu.ac.uk) for informal discussions.

## 2.

# NOVEL DRUG-DENDRIMER CONJUGATES AS NOVEL TREATMENTS FOR OVARIAN CANCER

According to the WHO, ovarian cancer occurred in 239,000 women in 2012, with 152,000 deaths associated with the disease. In the UK alone, ovarian cancer is responsible for the death of approximately 3000 women every year. Most patients are treated with chemotherapy, and often this is initially successful. However, many patients suffer a recurrence of their disease, and the tumour usually becomes resistant to treatment. Only 30% of women survive 5 years beyond diagnosis so there is a clear and present need to either develop new therapies to be used in place of chemotherapy, or which increase the effectiveness of chemotherapy, particularly in drug resistant disease. An emerging target for this disease is the enzyme, autotaxin. Many of autotaxin inhibitors discovered so far exhibit inadequate pharmacokinetic or pharmacodynamic properties that will impede their further development as drugs. In this highly interdisciplinary project we will investigate the development of a new series of therapeutics for the treatment ovarian cancer that have the potential to overcome the issues noted above. The project is based on (published) firm and unambiguous initial results and has real potential to deliver a drug candidate for clinical trials.

This project extends the existing and ongoing successful collaboration in oncology drug discovery between Prof. Steve Allin (NTU) and Dr. Alan Richardson (Reader in Pharmacology, Keele University) who will provide the pharmacological input and testing. All project needs are met within this collaboration.

### References

- WHO Cancer Report, 2014, Chapter 5.12. ISBN 9283204298.
- Allin, Richardson et al, Ovarian Cancer / Book 1, ISBN 978-953-307-812-0.
- Allin, Richardson et al, ACS Med. Chem. Lett, 2014, 5, 34.

**Supervisors:** Prof. Steve Allin, Prof. John Wallis and Dr. Alan Richardson

### Supervisor biogs

Prof. Steve Allin has supervised over 30 Ph.D. students leading to over 85 research publications. He has received external funding for his research >£2M awarded from the EPSRC, MRC, Leverhulme Trust and industrial partners. Allin co-founded (with Phil Page) Charnwood Molecular Ltd in 1998; the company now employs over 25 people, and has an annual turnover of over £1.8 million. Current h index = 26. Has a PhD completion rate of 94%.

Prof. John Wallis has published >130 research papers. Current h index = 20. Has a PhD completion rate of 100%.

Keele co-supervisor Dr. Alan Richardson, School of Pharmacy: has worked in the field of ovarian cancer for 12 years. The overall mission of his group is to identify drug targets and new drugs to treat ovarian cancer. His expertise in molecular pharmacology is particularly relevant to the proposed project.

**Entry Requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **chemistry, biochemistry or related subject**.

**Contact:** [steve.allin@ntu.ac.uk](mailto:steve.allin@ntu.ac.uk) for informal discussions.

### 3.

## ASSESSING INDICATORS AND MANAGEMENT CONDITIONS FOR PREDICTING POLYPHENOL CONTENTS IN WINE PRODUCTION

Flavonoids are a range of phenolic compounds present in plants serving different roles including flavouring. Flavonoids concentration in red wine depends on several factors including grape variety, cultivation area, sun exposure, enology technique and wine age<sup>1,2</sup>. Viticulturists currently measure quercetin (as a representative flavonoid) to characterize the sun exposure of vineyards and the impact of canopy management. However, comprehensive study on all the potential factors, including the variations in other important flavonoid compounds in wines, has yet to be attempted.

This study proposes to systematically study these influencing factors using a combination of instrumental analytical techniques, mathematical modelling and geographical information systems (GIS) spatial analysis. This will provide tools to enable management of the environment at vineyard level. A variety of grape and soil types will inform the analysis.

Instrumentally derived analytical data of soil, grape and wine flavonoid components will be derived using HPLC-DAD, LC-MS and total luminescence spectroscopy<sup>3,4</sup>. These and other environmental variables will build a database to which Bayesian belief networks and principal component analysis (PCA) will be applied to model the probability of the influencing factors<sup>4</sup>. GIS spatial analysis<sup>5, 6</sup> will permit interpretation of these factors with vineyard and environmental conditions.

### References

- Fang, F., Tang, K., & Huang, W. D. (2013). Changes of flavonol synthase and flavonol contents during grape berry development. *European Food Research and Technology*, 237(4), 529-540. doi: 10.1007/s00217-013-2020-z
- Gonzalez-Neves, G., Charamelo, D., Balado, J., Barreiro, L., Bochicchio, R., Gatto, G., Moutounet, M. (2004). Phenolic potential of Tannat, Cabernet-Sauvignon and Merlot grapes and their correspondence with wine composition. *Analytica Chimica Acta*, 513(1), 191-196. doi: 10.1016/j.aca.2003.11.042
- Seetohul, L.N., Scott, S.M., O'Hare, W.T., Ali, Z., Islam, M. (2013). Discrimination of Sri Lankan black teas using fluorescence spectroscopy and linear discriminant analysis, *J Sci Food Agric*, 93(9), 2308-14.
- Seetohul, L.N., Islam, M., O'Hare, W.T., Ali, Z. (2006) Discrimination of teas based on total luminescence spectroscopy and pattern recognition *J Sci Food Agric*, 86 (13) 2092 – 2098

**Supervisors:** Dr. Michael Coffey

### Supervisor biogs

Dr. Michael Coffey has experience in Analytical chemistry, Forensic Toxicology and Chemometrics. His own PhD relates to Novel Applications of Optical Analytical Techniques. As a forensic Toxicologist/Technical Manager at CFLM (Dundee), had primary responsibility for the management of the laboratory including the technical staff.

His keen interest in investigating novel ways at maximising recovery of analytical information from samples allowed him to carry out consultancy for several companies including Johnson Matthey & DuPont Teijin Films. As part of the Micro & Nanosystems group (Teesside University), was involved securing funding (€1.25 million) for a European project.

**Entry requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or a related discipline**.

**Contact:** [michael.coffey@ntu.ac.uk](mailto:michael.coffey@ntu.ac.uk) for informal discussions.

## 4.

# C-H FUNCTIONALIZATION FOR THE DIVERSE POST-SYNTHETIC MODIFICATION OF PEPTIDES AND PROTEINS

Methods for the direct post-synthetic modification of peptides and proteins at new sites in the biomolecule are in high demand. In this project, we will use transition metal catalyzed C-H functionalizations, reactions that are revolutionizing organic synthesis, to establish flexible methods for bioconjugation at unconventional sites. In particular, we are interested in modifying aromatic and heteroaromatic side chains of amino acid residues using direct C-C bond forming reactions.

The ultimate aim of the project is to develop versatile new tools for the post-synthetic modification of peptides and proteins with application in (a) advancing understanding of biological function, (b) diagnosis and treatment of disease, and (c) manufacture of new materials.

**Supervisors:** Dr. Warren Cross

### Supervisor biogs

This is a collaborative and interdisciplinary project: the student will be supervised by Dr Warren Cross (expertise in the area of C-H activation: (a) Cross et al. Chem. Eur. J. 2014, 20, 13203; (b) J. Org. Chem. 2014, 1954; (c) Chem. Comm. 2013, 1918) and will also work with Professor Carole Perry (expertise of working with peptides and proteins for a range of biomedical applications: Perry et al. (a) J. Am. Chem. Soc. 2012, 134, 6244; (b) Chem. Mater. 2014, 26, 5725; (c) Chem. Mater. 2014, 26, 2647). The student will also help to establish new collaborations (including outside NTU and internationally) to pursue further applications of the new bioconjugation techniques.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or related discipline**.

**Contact:** [warren.cross@ntu.ac.uk](mailto:warren.cross@ntu.ac.uk) for informal discussions.

## 5.

### C(SP3)-H ACTIVATION WITHOUT A DIRECTING GROU

Over the past decade a number of highly-efficient synthetic strategies have been developed that involve the use of a transition metal catalyst to directly cleave non-acidic C-H bonds, a process known as C-H activation.[1] These reactions are revolutionizing organic synthesis because they enable a more direct synthesis with fewer steps and because they enable unconventional synthetic strategies.

Two significant challenges in the field of C-H activation are the activation of C(sp<sup>3</sup>)-H bonds and C-H activation in the absence of a chelating directing group; we have achieved both of these transformations simultaneously, Scheme 1.[2] Moreover, this is a rare example of metal-ligand control of site-selectivity in C-H activation.

#### References

- L. Ackermann, Chem. Rev. 2011, 111, 1315–1345.
- W. B. Cross, S. Razak, K. Singh, A. J. Warner, Chem. Eur. J. 2014, 13203.

**Supervisors:** Dr. Warren Cross

#### Supervisor biogs

The student will be supervised by Dr Warren Cross, who has significant expertise in the area of C-H activation, see for example: (a) Cross et al. Chem. Eur. J. 2014, 20, 13203; (b) J. Org. Chem. 2014, 1954; (c) Chem. Comm. 2013, 1918.

#### Entry Requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or related discipline**.

**Contact:** [warren.cross@ntu.ac.uk](mailto:warren.cross@ntu.ac.uk) for informal discussions.

## 6.

# COMPUTATIONAL MODELLING OF BIOMOLECULE C-H FUNCTIONALIZATION REACTIONS

Methods for the direct post-synthetic modification of peptides and proteins at new sites in the biomolecule are in high demand. In this project, we will use high-level computational methods (density functional theory - DFT - and hybrid quantum mechanics / molecular mechanics – QM/MM) to model biomolecule functionalizations that involve a completely new type of reactivity: converting a C-H bond of an aromatic side chain to a robust C-C bond, Scheme 1.

In a related experimental project, we are establishing these reactions in the lab. This computational project will enable us to rationalize our experimental findings concerning reactivity and selectivity, especially relating to how the amino acid sequence and peptide structure affect the reactions. Moreover, the computational research will inform and direct the practical research. Crucially, there have been no reports on computational investigations of these types of reaction.

The ultimate goal of our research programme is to provide new enabling tools for biomedical research. Hence, we will also use MM and molecular dynamics (MD) calculations to probe the effects of the biomolecule modification on their function; specific applications will be determined by early work on the modifications possible and developed through new collaborations as appropriate.

**Supervisors:** Dr. Warren Cross

### Supervisor biogs

This is a collaborative and interdisciplinary project: the student will be supervised by Dr Warren Cross (expertise in the area of C-H activation: (a) Cross et al. Chem. Eur. J. 2014, 20, 13203; (b) J. Org. Chem. 2014, 1954; (c) Chem. Comm. 2013, 1918) and will also work with Professor Carole Perry (expertise of working with peptides and proteins for a range of biomedical applications: Perry et al. (a) J. Am. Chem. Soc. 2012, 134, 6244; (b) Chem. Mater. 2014, 26, 5725; (c) Chem. Mater. 2014, 26, 2647). The student will also help to establish new collaborations to pursue further applications of the new bioconjugation techniques.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or related discipline**.

**Contact:** [warren.cross@ntu.ac.uk](mailto:warren.cross@ntu.ac.uk) for informal discussions.



## 7.

### NEW TOOLS FOR DETECTION OF BIOLOGICAL AND FORENSIC EVIDENCES

In response to the need of continuous detection and monitoring of a variety of measurables that impact in our life such as water quality, pollution control, food and drinks composition, industrial manufacturing and medical diagnosis.

This project has the scope to sense many different targets but would initially be applied to the monitoring of water and waste water quality, additives in food and drinks, and forensic science using analytical techniques such as LC and GC-MS.

Once the target has been identified a specific host will be designed in order to increase sensitivity of an electrochemical sensor. The project will focus on the synthesis, characterisation and the study of binding ability of the host as well as its functionalisation to bind to the surface of a sensor.

**Supervisors:** Dr. Muriel Funck, Dr. Puddu and Dr. Smith

#### **Supervisor biogs**

The Director of Studies for the project, Dr Muriel Funck, Lecturer in Chemistry and Forensics joined the academic team at Nottingham Trent University in 2011. She is applying her background in synthetic and supramolecular chemistry to Forensic and environmental analysis.

Dr Puddu is a lecturer in inorganic chemistry. She has a track record in material synthesis, photocatalysis and materials' interfacial studies.

Dr Smith is a senior lecturer in physical chemistry, with expertise in electrochemistry, functional coating and surface characterization.

**Contact:** [muriel.funck@ntu.ac.uk](mailto:muriel.funck@ntu.ac.uk) for informal discussions.

## 8.

# ANTIMICROBIAL NANO-HYDROGEL WITH HEALING FUNCTIONS

This research addresses some urgent needs in medical field. Antimicrobial and healing functions are highly desirable in wound dressing materials. The current state-of-art of antimicrobial materials are essentially dominated by silver based biocides. The problem with silver based antimicrobial material is biocide leaching. The increased evidence on the toxicity of leached silver biocide has prevented this approach from wound dressing application. In addition, no any of the current state-of-art antimicrobial technology exhibits healing behaviour which is much needed in wound dressing products.

This project will investigate the feasibility to use nano-structured particles to form non-migration type of biocide and then to integrate the non-leaching biocidal nano-particles into hydrogel structure. The gel formed in this way will have permanent antimicrobial behavior without biocide leaching. The previous research at NTU has shown that it is possible to produce non-leaching types of antimicrobial nylon and polyolefin nanocomposites with healing functions for textiles, food and drink applications. The healing technology developed in our previous study will be introduced into the hydrogel system in this new project. The research will also investigate the enhancement of mechanical properties of the hydrogel by the nano-particles in order to enable the new material to be developed suitable for tough clinical and domestic application environment. Clinical assessment on the health and safety risk will be carried out in our collaborating partners' institutions.

**Supervisor:** Dr Fengge Gao

### Supervisor biogs

Dr. Fengge Gao is a Reader in Nanotechnology in the university. He has more than 30 years of research experience in a wide aspects of polymers and composite research with particular recent focus on filler enhanced polymer nanocomposites in property enhancement and new function development. He has been awarded over £1.5M external fund as Principal Investigator from the Royal Society, EPSRC, European Commission and global leading industries. Dr Gao is served as the member of UK Research Council EPSRC Peer Review College, member of SCI Fire and Materials Committee, also ex-executive of IET/IoN Microsystems and Nanotechnology Professional Network. His recent work on non-migration type of antimicrobial polymer nanocomposites won the CenFRA Most Innovative Research Award and UK Food and Drink Forum Innovation Champion Award.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **biology, chemistry or material science**.

**Contact:** [fengge.gao@ntu.ac.uk](mailto:fengge.gao@ntu.ac.uk) for informal discussions

## 9.

# NANO-STRUCTURED DIELECTRIC MATERIALS FOR ENERGY APPLICATION USING GEL COATING NANOTECHNOLOGY

One of the major challenges facing today is to ensure security of energy supply with minimum environmental impact. A central element of power systems is insulation. Consequently raising the efficiency of insulation in power devices plays an important role in tackling this challenge. It has been shown that a 0.2% efficiency increase in insulation materials could save the equivalent of 10 fossil fuel power plants and related reduction in CO<sub>2</sub> emission in the EU scale. The current state-of-art in improving the efficiency of insulation materials is through the enhancement of breakdown behavior of dielectric materials by dispersing dielectric nano-fillers into the materials to diversify the development of charging path and to increase the length of the path development. Our previous EU Anastasia project already pushed this into a very high level by improving the breakdown strength by more than 50%.

This new project is aimed to raise the level into a new dimension by fundamentally changing the structure of the insulation through introducing continuous nano-mineral layer on the surface of insulation devices using gel coating nanotechnology. Our preliminary study has shown that it is possible to form a continuous nano-mineral thin layers through gel coating technology on the surface of solid polymers. This project will apply this technology into dielectric tapes and high field insulation devices. The continuous insulation nano-coating layer will be more effective in preventing electric breakdown with flexibility to tailor the material into non-linear conduction behavior to introduce grading functions.

**Supervisors:** Dr. Fengge Gao

### Supervisor biogs

Dr. Fengge Gao is a Reader in Nanotechnology in the university. He has more than 30 years of research experience in a wide aspects of polymers and composite research with particular recent focus on filler enhanced polymer nanocomposites in property enhancement and new function development. He has been awarded over £1.5M external fund as Principal Investigator from the Royal Society, EPSRC, European Commission and global leading industries. Dr Gao is served as the member of UK Research Council EPSRC Peer Review College, member of SCI Fire and Materials Committee, also ex-executive of IET/IoN Microsystems and Nanotechnology Professional Network. His recent work on non-migration type of antimicrobial polymer nanocomposites won the CenFRA Most Innovative Research Award and UK Food and Drink Forum Innovation Champion Award.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Physics, Materials Science, Chemistry or Chemical Engineering**.

**Contact:** [fengge.gao@ntu.ac.uk](mailto:fengge.gao@ntu.ac.uk) for informal discussions.

## 10.

# NOVEL STAIN-FREE MATERIALS WITH ABILITY TO ABSORB MOISTURE

The current state-of-art of stain-free fabrics is developed based on super hydrophobic principle to introduce either low surface energy coating or micro and nano particle enhanced hydrophobicity to achieve repellent behaviour. However such a material does not have the ability to absorb moisture which is one of the key factors to determine if a cloth is comfortable. A breakthrough has been made in our Nanoscience Laboratory towards understanding the mechanisms of natural species who have both stain repellence behaviour and the ability to absorb moisture. This PhD project will mimic the principles obtained from our previous study to develop new synthetic material system which have similar properties and functions.

### References

- F. Gao, E. Baraka-Kamali, N. Shirtcliffe, C. Terrell-Nield, A preliminary study of the surface properties of earthworms and their relations to non-stain behaviour, Journal of Bionic Engineering, 7, 13-18, 2010.

**Supervisors:** Dr. Fengge Gao

### Supervisor biogs

The Director of Studies for the project is Fengge Gao who is a Reader in Nanotechnology. Dr. Gao has more than 30 years of research experience in structure enhancement and function creation of polymer and composite materials. Since joining Nottingham Trent University in 1998, Dr. Gao's work on property and function enhancement of materials has been awarded over £1.5M external fund from the Royal Society, EPSRC, EU FP7, BAE Systems, Alcoa USA, Hilti AG, Colormatrix, Alstom AG and many other global leading industries and organisations. The applications of these research cover beverage packaging, aerospace, energy, fire retardancy and antimicrobial fields. Dr Gao is currently served as the member of UK Research Council EPSRC Peer Review College. His recent work on non-migration type of antimicrobial polymer nanocomposites and hygiene surface coating in food and drink environment won the CenFRA Most Innovative Research Award and also UK Food and Drink Forum Innovation Champion Award 2009.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry, physics or material science**.

**Contact:** [fengge.gao@ntu.ac.uk](mailto:fengge.gao@ntu.ac.uk) for informal discussions.

## 11.

# ULTRA-LIGHT THERMAL AND OXIDATION RESISTANT MATERIALS

Ultra-light weight materials are highly desirable in aerospace, automotive and building industries. The recent development of graphene and carbon nanotube based ultra-light weight foams has showed promising in pushing foam density further lower and opening up wider applications. The problem with carbon based foam is weak oxidation resistance in air environment. In order to overcome this difficulty, this PhD project will develop thermal and oxidation resistance ultra-light foams with desired mechanical properties. The advance in this research would have great impact on future transport, energy saving, aerospace, fire protection and building and architecture fields.

### References

- F. Gao, Clay/Polymer Nanocomposites, the story, *Materials Today*, 7(11), 50-55, 2004.
- F. Gao, G. Beyer, G and W. Yuan, A mechanistic study of fire retardancy of carbon nanotube/ethylene vinyl acetate copolymers and their clay composites, *Polymer Degradation and Stability* 89, 559-564, 2005.
- F. Gao, J.W. Patrick and A. Walker, "Multiple CVD Densification of PAN-Based Carbon-Fibre Reinforced Carbon Laminates", *Carbon*, 32, 1215-1222, 1994.
- F. Gao, J.W. Patrick and A. Walker, "The Characterisation of Cracks and Voids in 2-D Carbon/Carbon Composites", *Carbon*, 31, 103-108, 1993.

**Supervisors:** Dr. Fengge Gao

### Supervisor biogs

The Director of Studies for the project is Fengge Gao who is a Reader in Nanotechnology. Dr. Gao has more than 30 years of research experience in developing light-weight carbon based materials including processing of carbon fibres and carbon fibre reinforced carbon composites. He is also active in fire retardancy and nanocomposite research. Since joining Nottingham Trent University in 1998, Dr. Gao has been awarded over £1.5M external fund. Dr Gao is currently served as the member of UK Research Council EPSRC Peer Review College. His recent work on non-migration type of antimicrobial polymer nanocomposites and hygiene surface coating in food and drink environment won the CenFRA Most Innovative Research Award and also UK Food and Drink Forum Innovation Champion Award 2009.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry, Material Science, Chemical Engineering, Physics**.

**Contact:** [fengge.gao@ntu.ac.uk](mailto:fengge.gao@ntu.ac.uk) for informal discussions.

## 12.

### DIPEPTIDES FOR TREATING DIABETES

Diabetes is the 8th largest killer disease in the world, with 3.2 million cases diagnosed in the UK and many more worldwide. New treatments to alleviate insulin deficiency are required and this medicinal chemistry project involves the design and synthesis of a targeted libraries of  $\alpha/\beta$ -dipeptides (Figure 1) for screening in a collaborative project, seeking new treatments for diabetes.

The project will encompass in silico design and screening of potential drug leads along with synthesis, characterisation of biological testing of compound libraries. This project offers multidisciplinary training in synthetic chemistry, computational drug discovery, biochemistry and cell biology - vital skills for further research at the chemistry/biology interface.

**Supervisors:** Dr. Chris Garner

#### **Supervisor biogs**

The project will be supervised by Dr Chris Garner, an Organic Chemist with a track record and expertise synthetic in medicinal chemistry, and Dr Mark Turner a Reader in Biochemistry with specialist expertise in type 2 diabetes. The candidate undertaking this project will work within the two research groups, located adjacent to one another, and will receive extensive training in all aspects of the work.

#### **Entry requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or related discipline**.

**Contact:** [Christopher.garner@ntu.ac.uk](mailto:Christopher.garner@ntu.ac.uk) for informal discussions.

## 13.

### KINETIC RESOLUTION STRATEGIES FOR CHIRAL SECONDARY PHOSPHINE OXIDES

P-chirogenic phosphine ligands are exceptional in conferring high levels of stereoselectivity in a wide variety transition metal mediated processes, whilst the utility of P-chirogenic phosphine oxides has yet to be exploited. The current methodology for the preparation of P-chiral secondary phosphine oxides is very limited and this project will examine new methods for the preparation of these materials in enantiopure form. This project will explore the kinetic resolution of the, little known, acylphosphine oxides using chiral nucleophiles (Figure 1). Previous work in the Garner group has established robust routes to these compounds and explored their reactivity. This project provides training and experience in the challenging field of asymmetric synthesis and provides an excellent grounding for anyone wishing to pursue a career in synthetic chemistry.

**Supervisors:** Dr. Chris Garner

#### **Supervisor biogs**

The project will be supervised by Dr Chris Garner an organic chemist with a long track record in asymmetric synthesis of amine and natural products and will be co-supervised by Prof. John Wallis whose group has interests in the synthesis of organic conductors, heterocycles and anti-cancer agents.

#### **Entry Requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or related discipline**.

**Contact:** [Christopher.garner@ntu.ac.uk](mailto:Christopher.garner@ntu.ac.uk) for informal discussions.

## 14.

# THE ANALYSIS OF LARGE CLUSTERS BY FLUORESCENCE ANISOTROPY

Aggregation phenomena is important in a wide range of biological processes. These include the formation of clusters during receptor activation and the formation of plaques causing cataracts and dementia.

Fluorophores can report on cluster formation due to them undergoing a range of photophysical processes including energy transfer and quenching. In molecules labeled with a single fluorophore (e.g. fluorescein) energy transfer results in a reduction in the fluorescence anisotropy upon clustering.

Previous work on induced assembly and exhaustive labeling of proteins has shown that the size of fluorophore clusters (including large clusters of  $n > 20$ ) should be accessible to analysis using fluorescence anisotropy assuming the right combination of quenching and fluorescence enhancement is created.

The project contains a synthetic component and an analysis component. The synthetic component will create amine reactive dyes containing anthracene, and perylene type dyes which are known to exhibit enhanced fluorescence through exciplex formation. The analysis component will include use of these new fluorophores and others to assess the photophysical properties of clusters and assemblies.

### References

- Gholami, Z. and Q. Hanley. Controlled Assembly of SNAP-PNA-Fluorophore systems on DNA Templates to Produce Fluorescence Resonance Energy Transfer. *Bioconjugate Chemistry*, 25:1820-1828 (2014).
- Zolmajd-Haghighi Z. and Q. S. Hanley. When One Plus One Does Not Equal Two: Fluorescence Anisotropy in Aggregates and Multiply Labeled Proteins, *Biophysical Journal*, 106(7):1457-1466 (2014).
- Gholami Z., L. Brunsveld, and Q. S. Hanley. PNA-Induced assembly of fluorescent proteins using DNA as a framework, *Bioconjugate Chemistry*, 24(8):1378–1386 (2013).

**Supervisors:** Dr. Quentin Hanley

### Supervisor biogs

Dr. Quentin S. Hanley is a Reader in Analytical Chemistry and Dr. Chris Garner is a Senior Lecturer in Organic Chemistry. Between them they have the expertise to carry out this research. Together they supervised to completion Dr Zahra Gholami (See references 1 and 3 above).

Dr Hanley was Head of Chemistry and Forensics at NTU from 2008 to 2011 and teaches aspects of Chemistry, Forensic Science and Physics. His independent research work has made contributions to imaging, data analysis and visualization, chemical education, fluorescence dynamics, and biophysics and he has further research experience in chemical oceanography, environmental health, x-ray imaging, applications of synthetic biology to template driven assembly, microscopy, and criminology. In the area of



microscopy, he has been awarded 4 patents. Dr. Hanley is an author or co-author on over 50 peer-reviewed papers and has been involved in projects receiving total funding in excess of £2M from EPSRC, EU, RSC, and industry.

**Entry requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **chemistry, or related subject**.

**Contact:** [quentin.hanley@ntu.ac.uk](mailto:quentin.hanley@ntu.ac.uk) for informal discussions.

## 15.

### WATER BASED COATINGS FOR PHARMACEUTICAL DOSAGE FORMS

Sustained and controlled release of drugs can be achieved by the coating of drug cores with aqueous film forming polymer latex particles. Solute transfer through these films can occur by solution/diffusion through the bulk polymer or through aqueous pathways in the porous film structure or a combination of the two. Aqueous pathways may develop as the emulsifier residues arising from the emulsion polymerisation process of latex production leach out. Polymer latex particles can however be produced by emulsifier-free emulsion polymerisation to give greater control over this transport route for the solute drug although this approach has yet to be fully explored and commercially developed. The process could be further developed to make use of the potential of the latex to offer catalytic functional groups (1) so that a pro-drug could be employed which would be converted to its active form only after passage through the latex film. This would avoid the potential hazard in sustained release formulations of massive overdosing if the dosage form is compromised by damage for example by chewing.

Typically drug core beads can be produced by blending the drug with cellulose excipient and extruding and spheronizing. Latex coating is then applied by atomized spraying of wet latex onto the drug cores in a heated fluidized bed. This can be on a bench top scale and can be supported at the earlier stages of development by 'pan coating' by dropwise addition of latex on to a heated rotating pan of drug cores.

Sustained/controlled release performance can be tested in conventional in-vitro drug dissolution equipment with concentrations monitored by spectrophotometry in flow-through cells.

This study would centre around the performance of surfactant-free polymer latex particles both as homopolymer and core-shell particles and the effects of temperature and time on film performance in drug permeation.

#### References

- Ian C Hodges and John Hearn Reactive Latex Films Langmuir 2001, 17, 3419-3422

**Supervisors:** Dr. John Hearn

#### Supervisor biogs

Dr John Hearn is Reader in Colloid Science at NTU and over a 40 year career has supervised and externally examined PhD students and published peer reviewed papers on polymer latex particles and polymer latex films and related surface and colloid chemistry topics.

#### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or related discipline**.

**Contact:** [john.hearn@ntu.ac.uk](mailto:john.hearn@ntu.ac.uk) for informal discussions.

## 16.

### COMPOSITE THIN POLYMER LATEX FILMS

A thin coating of latex can protect substrates from oxygen and water vapour ingress or alternatively be used to control solute permeation rates (1,2). Multi layered films can be produced with a top coat of the more expensive or functionally active component. Monolayer coverage can be achieved with a Langmuir Blodgett technique to influence surface hydrophobicity

Thin, 10 micron scale, polymer latex films can be prepared by 'flash casting' when wet latex is sprayed on to a heated surface such as a PTFE coated steel block and water quickly evaporates.

A free latex film can then be recovered from the surface so that its permeability properties can be studied. Side differences can be examined with regard to film/substrate and film/air interfaces. In situ films can also be prepared in this manner onto for example a compact powder of potential permeant.

#### References

- Ian C Hodges and John Hearn Reactive Latex Films Langmuir 2001, 17, 3419-3422
- Paul A Steward, John Hearn and Michael C Wilkinson An overview of polymer latex film formation and properties Advances in Colloid and Interface Science 2000, 86, 195-267

**Supervisors:** Dr. John Hearn

#### Supervisor biogs

Dr John Hearn is Reader in Colloid Science at NTU and over a 40 year career has supervised and externally examined PhD students and published peer reviewed papers on polymer latex particles and polymer latex films and related surface and colloid chemistry topics.

#### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or related discipline**.

**Contact:** [john.hearn@ntu.ac.uk](mailto:john.hearn@ntu.ac.uk) for informal discussions.

## 17.

# DEVELOPING A HIGH CONFIDENCE MULTIPLEXED ASSAY FOR PROTEIN TOXINS FOR FOOD SECURITY

Food products and ingredients are transported in large volumes and it is therefore important to develop screening methods to confirm that the material is not contaminated by toxins that would be dangerous if consumed. Many toxins are small molecules and there are already good screening methods for them. However, bacterial toxins (and some of plant origin) are large protein molecules that are harder to analyse. Screening methods for these do exist, but they are complex assays that limit throughput. This project will seek to develop a method and instrumental screening tool whereby large toxin molecules present in foodstuff are selectively pre-concentrated (using molecular recognition elements), enzymatically fragmented and analysed in an online fashion, using newly developed LC columns and mass spectrometry, with a view to defining a system that could be used for high throughput, high confidence screening in an industrial environment. The project will include method development, instrument development and bioinformatics approaches to meet the goal. The aim will be to identify the simplest, cheapest, most robust system that could be developed but that would still meet the confidence levels required.

### References

- Careri, M., F. Bianchi, and C. Corradini. 2002. Recent advances in the application of mass spectrometry in food-related analysis. *Journal of Chromatography A* 970 (1–2) (9/13): 3-64.
- Lee, Su Jin et al. 2014. Aptamer/ISET-MS: A new affinity-based MALDI technique for improved detection of biomarkers. *Analytical Chemistry* 86 (15) (08/05): 7627-34.
- Ler, Siok Ghee et al. 2006. Trends in detection of warfare agents: Detection methods for ricin, staphylococcal enterotoxin B and T-2 toxin. *Journal of Chromatography A* 1133 (1–2) (11/10): 1-12.
- Madian, Ashraf G. et al. 2013. Mass-linked immuno-selective assays in targeted proteomics. *Analytical Chemistry* 85 (2) (01/15): 737-48.
- Nedelkov, Dobrin et al. 2000. Multitoxin biosensor–mass spectrometry analysis: A new approach for rapid, real-time, sensitive analysis of staphylococcal toxins in food. *International Journal of Food Microbiology* 60 (1) (9/15): 1-13.

**Supervisors:** Dr. David Kilgour

### Supervisor biogs

Dr Kilgour has broad expertise in the field of applied mass spectrometry. He has undertaken research in advanced mass spectrometric development at the Universities of Edinburgh and Warwick in the UK and the University of Maryland Baltimore, in the US and now undertakes his research at Nottingham Trent University – a university with an excellent reputation in the area of mass spectrometry. He has also worked outside academia and was a scientist with the Ministry of Defence for 8 years. He has mentored graduate students in Austria, France, the UK and the US.

Dr Coffey provides experience in the field of applied analysis and has worked for UK universities, for government analytical laboratories and private consultancies developing and assessing assays for in-the-field use. He has mentored a number of graduate students at Nottingham Trent University.

**Entry requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry, biochemistry**.

**Contact:** [david.kilgour@ntu.ac.uk](mailto:david.kilgour@ntu.ac.uk) for informal discussions.

## 18.

# A NEW, NOVEL LIQUID INTERFACE FOR MASS SPECTROMETRY

Electrospray ionisation (and related techniques such as nanospray) allowed mass spectrometry to analyse bio-macromolecules such as proteins. This capability has become a key cornerstone of biomedical research. Whilst electrospray and nanospray analyses provide excellent performance, they do have inherent weaknesses. This project will involve the development of a new type of liquid interface for mass spectrometry. This liquid ion source will allow gas phase ions to be generated from very small liquid volumes (perhaps down to the volume of a single cell) and will automatically monitor the resulting mass spectra and will adapt its performance to match the concentration of the sample. It will also allow sample solutions and standards to be mixed and ionised in real time to ensure that the mass spectra have the optimum mass accuracy (and hence the confidence we can have in the assignments). And, it will be designed to couple to robotic liquid handling systems.

### References

- Fenner and McEwen. 2015. Survival yield comparison between ESI and SAIL: Mechanistic implications. *International Journal of Mass Spectrometry* 378 (2/15): 107-12.
- Forbes. 2015. Rapid detection and isotopic measurement of discrete inorganic samples using acoustically actuated droplet ejection and extractive electrospray ionization mass spectrometry. *Rapid Communications in Mass Spectrometry* 29 (1): 19-28.
- Forbes et al. 2007. Multiplexed operation of a micromachined ultrasonic droplet ejector array. *Review of Scientific Instruments* 78 (10): 104101.
- Goodlett et al. 2014. Development of a surface acoustic wave nebulization source for mass spectrometry. Paper presented at Abstracts of the 248th American Chemical Society Fall National Meeting.
- Hommersom et al. 2016. An ambient detection system for visualization of charged particles generated with ionization methods at atmospheric pressure. *Rapid Communications in Mass Spectrometry* 30 (3): 352-8.

**Supervisors:** Dr. David Kilgour

### Supervisor biogs

Dr Kilgour has broad expertise in the field of applied mass spectrometry. He has undertaken research in advanced mass spectrometric development at the Universities of Edinburgh and Warwick in the UK and the University of Maryland Baltimore, in the US and now undertakes his research at Nottingham Trent University – a university with an excellent reputation in the area of mass spectrometry. He has also worked outside academia and was a scientist with the Ministry of Defence for 8 years. He has mentored graduate students in Austria, France, the UK and the US.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st

Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **chemistry, biochemistry, physics**.

**Contact:** [david.kilgour@ntu.ac.uk](mailto:david.kilgour@ntu.ac.uk) for informal discussions.



## 19.

### NEW APPROACHES TO STUDYING BIOMOLECULE-MATERIAL INTERACTIONS

Biomaterials such as bone, teeth, seashells and the hard parts of grasses and plants are wonderful examples of the power of living organisms to construct functional composite materials. The materials generated are far superior to those we can currently make in the laboratory and they are made under mild (ambient) synthesis conditions using biomolecules such as proteins/ lipids/ carbohydrates in combination with simple oxides and salts including silica, calcium carbonate and calcium phosphate. It is important that we understand the interface between the biotic (biomolecule) and abiotic (mineral) phase as this is key to the practical success of the biomaterial and will help us in the design of superior composite materials for biomedical and other industry focused applications.

This project will advance our understanding of the biomolecule material interface by the development of new tools to study biomolecules on surfaces of particles. The project will comprise both experimental and computational aspects. The experimental work will develop new approaches using techniques such as fluorescence and Raman spectroscopies and thermal methods such as isothermal titration calorimetry. The new approaches will be complemented by quantitative assessment of biomolecule material binding by established chemical and biochemical assays. Molecular dynamics calculations will be used both to explain experimental results and to assist in the design of experiments by, for example, predicting modes of binding, biomolecule conformation/ conformation change on binding.

**Supervisors:** Prof. Carole Perry

#### Supervisor biogs

The Director of Studies is Carole C. Perry (MA (Oxon), DPhil (Oxon)) who is a Professor of Bioinorganic and Materials Chemistry. She is the holder of a Royal Society Wolfson Research Merit award (2013-2017) for recognition of the excellence of her research. Prof. Perry joined Nottingham Trent University in 1993 from a Lectureship in Inorganic Chemistry at Brunel University. Prior to that she held the EPA Brereton-Sherman junior research fellowship at St Hilda's College, Oxford University. She recently spent the academic year 2012-2013 at the Radcliffe Institute for Advanced Study, Harvard University. She has held visiting fellowships/ professorships at the Weizmann Institute for Science, the Scripps Institute for Oceanography, Université Pierre et Marie Curie and Universität Karlsruhe.

Prof. Perry has lead supervised 26 Doctoral Research students to successful completion. Past students work in academia or hold senior posts in nanotechnology/ biotechnology firms worldwide.

#### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **chemistry or related subject**.

**Contact:** [carole.perry@ntu.ac.uk](mailto:carole.perry@ntu.ac.uk) for informal discussions.

## 20.

# TiO<sub>2</sub> BASED HETERO-STRUCTURES FOR SOLAR LIGHT TECHNOLOGIES

In this project we aim to design innovative hierarchical hetero structures, containing TiO<sub>2</sub>, where each component utilizes different parts of the solar spectrum, with the final aim of improving overall adsorption properties. Synthesis and characterization of TiO<sub>2</sub> from an unusual precursor will be investigated using established hydrothermal and sol-gel synthetic routes, with a focus on the effect of different surfactants/additives on material's morphology and structure. We aim to verify the feasibility of a similar synthetic approach for the preparation of a selection of near-infrared and visible light absorbers in nanoparticulate form.

Since the contact between the different components can affect the light utilization properties of the material we also aim to study the effect of the integration of material components at the nanoscale, in contrast to micro-scale systems. Our findings will guide the intentional design of an optimal integrated photocatalysts for environmental and energy technologies.

**Supervisors:** Dr. Valeria Puddu

### Supervisor biogs

Dr Puddu has presented or co-authored over 20 conferences proceedings of specialized materials and photocatalysis meetings including two Keynote talks (EuroBioMat 2011, AOT-15 2009).

She is currently applying her expertise in photocatalysts synthesis to develop novel materials with improved absorption properties that can find applications in energy production (photovoltaics), energy storage (molecular fuels) and photoreduction of CO<sub>2</sub>. Dr Puddu has ongoing collaborations at NTU and other universities on projects associated with the development and testing of these systems.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry, Chemical Engineering or related discipline**.

**Contact:** [valeria.puddu@ntu.ac.uk](mailto:valeria.puddu@ntu.ac.uk) for informal discussions

## 21.

### TiO<sub>2</sub> STRUCTURES FOR SOLAR LIGHT TECHNOLOGIES

Titania (TiO<sub>2</sub>) is important photocatalytic material, with an established role in environmental remediation. It is currently used in the development of solar cells alternative to traditional solar panels. However, TiO<sub>2</sub> can only absorb UV light, and therefore utilize less than 5% of the light impinging on the Earth's surface. Adsorption properties of TiO<sub>2</sub> are typically improved by adding dopants or organic dyes, or other semiconductors. In this project we will investigate strategies to improve light absorption and utilizes a wide range of the solar spectrum, with a particular focus on the NIR region. This project builds on established synthetic routes applied on recently discovered near-infrared and visible light absorbers and entails both material preparation and characterization; providing an opportunity to develop a wide range of skills relevant to material chemistry aimed at specific technological applications.

**Supervisors:** Dr. Valeria Puddu

#### **Supervisor biogs**

Dr Puddu is a lecture in inorganic chemistry. She has a track record in material synthesis, photocatalysis, and materials' interfacial studies. Relevant publication can be found in the top ranking catalysis and material chemistry journals. Example include: Applied Catalysis B, Environmental (IF: 6.4); ACS Nano (IF: 12); Chemistry of Materials (IF: 8.5).

Dr Puddu is currently applying her expertise in photocatalysts synthesis to develop materials with improved absorption properties that can find applications in energy production (photovoltaics), energy storage (molecular fuels), photoreduction of CO<sub>2</sub>. Dr Puddu has ongoing collaborations at NTU and other universities on projects associated with the development and testing of these systems.

#### **Entry requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry, Chemical Engineering or related discipline**.

**Contact:** [valeria.puddu@ntu.ac.uk](mailto:valeria.puddu@ntu.ac.uk) for informal discussions.

## 22.

# TiO<sub>2</sub> NANOMATERIALS FOR ELECTROCHEMICAL SENSING

There is a growing need for continuous detection and monitoring of a variety of measurables that impact in our life, such as: water quality, pollution control, food and drinks composition, industrial manufacturing and medical diagnosis. TiO<sub>2</sub> is a promising candidate for the development of good sensors due to its low cost and the extent of control over physical properties like its surface area and morphology. One dimensional morphologies like nanorods and nanotubes have shown very promising results. TiO<sub>2</sub> offers advantages compared to other materials, thanks to the photocatalytic processes occurring at its surface that can be channelled to drastically improve the electrode analytical response and detection limits. TiO<sub>2</sub> electrochemical sensors are successfully used only for non-selective applications such as the determination of total organic matter (e.g.: COD) in water. We are interested in assessing the feasibility of this technology for the development of selective systems by investigating specific surface functionalisation.

This project has the scope to sense many different target analytes but would initially be applied to the monitoring of water and wastewater quality, with potential expansion to the study of additives in food and drinks, and forensic relevant compounds.

**Supervisors:** Dr. Valeria Puddu

### Supervisor biogs

Dr Puddu is a lecturer in inorganic chemistry. She has a track record in metal oxide nanostructures, TiO<sub>2</sub> photocatalysis and materials' interfacial studies. Relevant publication can be found in the top ranking catalysis journal (Applied Catalysis B, Environmental IF: 6.4) and in high quality material chemistry journals (ACS Nano: IF: 12; Chemistry of Materials IF: 8.5). Dr Puddu will supervise the design and preparation of the sensing material.

Dr Smith is a lecture in physical chemistry, with expertise in electrochemistry, functional coating and surface characterization. Dr Smith will support the set up and test of sensing device.

Dr Funck is a lecturer in forensic chemistry with expertise in supramolecular chemistry and analysis of biological and forensic evidence. Dr Funck will assist with the analytical aspects of the project including the application to forensic analysis.

### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **chemistry, chemical engineering**.

**Contact:** [valeria.puddu@ntu.ac.uk](mailto:valeria.puddu@ntu.ac.uk) for informal discussions.

## 23.

### LEGAL HIGHS ARE THEY LEGAL?

The growth of Novel Psychoactive Substances (NPS) (commonly known as Legal Highs and/or Research Chemicals) over the last decade, both in terms of availability and consumption, is of increasing public health concern. The number of new NPS reported to the European Monitoring Centre for Drugs and Drug Addiction (EMCDDA) has increased year on year from 41 in 2010 to 81 in 2013 with over 350 substances now being monitored (EMCDDA, 2014). In addition, the United Nations Office on Drugs and Crime (UNODC) estimates that a total of 348 NPS had been identified by member states by mid-2013 (UNODC, 2014).

The scale of NPS use globally is obscure due to an absence of epidemiological data from large population based samples and only limited data from a few countries on specific substances. Differences in legislation in different countries further complicate the ability to accurately understand use within and across countries.

Most research to date on NPS-related harms is in relation to fatal poisonings and limited to deaths involving specific drugs.

This study proposes to systematically characterise commercially available NPS and investigate their stability in biological matrices and embalming fluids. This will provide practitioner in Forensic Toxicology and the medical community with important information that would help with identification and interpretation of metabolites of these NPS

Instrumentally derived analytical data of NPS will be derived using HPLC-DAD, LC-MS, GC-MS and NMR. . Research on these substances has the potential to contribute significantly and help alleviate the lack of published information dealing with NPS. The field will appreciate any interesting data and this may be useful for medical practitioners.

All analytical instrumentation and sample preparative facilities and all required software are currently available at NTU.

**Supervisors:** Dr. Nitin Seetohul

#### **Supervisor biogs**

The Director of Studies for the project is Dr Nitin Seetohul who is a Senior lecturer in Analytical Chemistry and Forensics. Dr Nitin Seetohul has a BSc Chemistry, MSc in Analytical Chemistry and PhD in Novel Applications of Optical Analytical Techniques. Dr Seetohul joined Nottingham Trent University in 2013 from Forensic Toxicologist/ Lecturer at the University of Dundee. As a Case Active Forensic Toxicologist for Scottish Crown Office (2010-2013) he had primary responsibility for the management of the toxicology laboratory and technical staff that provided analysis of various post-mortem samples. Project Officer (2006-2008) on EU funded projects managing analytical chemistry support to SMEs in North East England. As part of this remit carried out stability testing and characterisation of a product to ensure an SME could meet rigorous European Union legislation.

#### **Entry requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree

(or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry, Biomedical Sciences or related subject**.

**Contact:** [nitin.seetohul@ntu.ac.uk](mailto:nitin.seetohul@ntu.ac.uk) for informal discussions

## 24.

### **MATERIALS CHEMISTRY: THE DEPOSITION OF ANTIMONY FROM DEEP EUTECTIC SOLVENTS (DESS)**

Deep Eutectic Solvents (DESS) are a class of ionic liquid which have great potential as alternative and more environmentally benign solvents for metal plating. This project targets promising new metal plating technologies involving DESS. These highly tuneable ionic liquids have been proven to be suitable for the deposition of a range of metals and are alternatives to conventional aqueous or organic solvents. The understanding and improvement of the plating process in DESS is an area of industrial importance for the electronics, automotive and aerospace sectors. An emerging area of industrial importance is the use of antimony in microelectronics.

Fundamental studies will be carried out to improve understanding of the antimony plating process using electrochemical methods alongside other surface analysis techniques such as scanning electron microscopy with energy dispersive x-ray analysis and atomic force microscopy. This project will investigate a range of DESS as 'greener' and more environmentally friendly solvent systems for plating antimony. The effect of changing DES; plating conditions (both electroless and electrochemical: galvanostatic, chronoamperometric, potentiodynamic); and substrate (both conducting metal pieces and non-conducting surfaces such as plastic) on the morphology of the coating will be investigated.

#### **References**

- Smith, E. L.; Abbott, A. P.; Ryder, K. S. Chem. Rev. 2014. DOI: 10.1021/cr300162p
- Smith, E. L.; Barron, J. C.; Abbott, A. P.; Ryder, K. S., Anal. Chem. 2009, 81, 8466–8471. DOI: 10.1021/ac901329e
- Abbott, A.P.; Griffith, J.; Nandhra, S.; O'Connor, C.; Postlethwaite, S.; Ryder, K. S.; Smith, E. L. Surface & Coatings Technology, 2008, 202, 10, 2033-2039. DOI: 10.1016/j.surfcoat.2007.08.055

**Supervisors:** Dr. Emma Smith

#### **Supervisor biogs**

This project will be based in the Chemistry and Forensic Team and will be led by Dr Emma L. Smith, a recent appointment at NTU, and first author of a current review into the applications of deep eutectic solvents. She has interests in surface analysis, metal plating, deep eutectic solvents and conducting polymer materials. Dr Lee Martin (inorganic chemistry) will be the second supervisor for the project. The person undertaking this project will be exposed to different aspects of materials chemistry and surface analysis with a strong focus on the industrial application of the research. Students will be encouraged to present their research locally and at international conferences. Training in experiments, theory and research methodology will be provided.

#### **Entry requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st



Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or related discipline**.

Contact: [emma.smith@ntu.ac.uk](mailto:emma.smith@ntu.ac.uk) for informal discussions.

## 25.

### THE DESIGN OF NEW ELECTROCHEMICAL SENSORS

There is a continuous need for the detection and monitoring for a variety of analytes that can impact on our life in areas such as water quality, pollution control, food and drinks composition, industrial manufacturing and medical diagnosis.

This project concerns the design, investigation and development of suitable electrochemical sensors and photosensor technology of high selectivity, to identify target analytes for the monitoring of the quality of water and waste water; determining additives in food and drink.

The person undertaking this project will be exposed to different aspects of materials chemistry and surface analysis with a strong focus on the industrial application of the research. Students will be encouraged to present their research locally and at international conferences. Training in experiments, theory and research methodology will be provided.

**Supervisors:** Dr. Emma Smith

#### **Supervisor biogs**

The Director of Studies for the project, Emma Smith (BSc, DPhil), is a Senior Lecturer in Chemistry and Forensics. Dr Smith joined Nottingham Trent University at the end of 2012 and specialises in electrochemistry she is an author or co-author of 15 peer-reviewed papers.

Dr Funck is a lecturer in forensic chemistry with expertise in supramolecular chemistry and analysis of biological and forensic evidence. Dr Puddu has presented or co-authored over 20 conference proceedings of specialized materials and photocatalysis meetings including two Keynote talks (EuroBioMat 2011, AOT-15 2009).

#### **Entry requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **chemistry or related subject**.

**Contact:** [emma.smith@ntu.ac.uk](mailto:emma.smith@ntu.ac.uk) for informal discussions.

## 26.

### SYNTHESIS OF LIBRARIES FOR BIOLOGICAL TESTING BASED ON NOVEL HETEROCYCLIC CHEMISTRY

This project is focused on developing reactions to new heterocyclic systems, which have never been made before, and which are of interest to the pharmaceutical industry.<sup>1,2</sup> The project will concentrate on reactions of highly electrophilic species, e.g. families of alkynes, allenes, chiral cyclic sulfate esters such as 1-3 and related materials with a great variety of poly-nucleophiles, e.g. thioureas and hydrazines to provide a range of new ring systems. The project will be guided in part by the need to expand the range of heterocyclic systems available and the need to move away from planar systems as drug candidates<sup>1,2</sup>. The overall aim is to produce a commercial library of such materials for use by the pharmaceutical industry in their searches for new lead compounds against various medical conditions. The design of new libraries is a topic of great current interest.<sup>3</sup> This project has a degree of freedom to explore new chemistries.

#### References

- W.R. Pitt, D.M. Parry, B.G. Perry, C.R. Groom, J. Med. Chem., 2009, 52, 2952; DOI: 10.1021/jm801513z
- F. Lovering, J. Bikker, C. Humblet, J. Med. Chem., 2009, 52, 6752; DOI: 10.1021/jm901241e.
- P.J. Hajduk, W.R.D. Galloway, D.R. Spring, Nature, 2012, 470, 42; S. Dandapani, L.A. Marcaurelle, Curr. Opinion Chem. Biol., 2010, 14, 362.

**Supervisors:** Prof. John Wallis

#### Supervisor biogs

The project will be led by Professor John D. Wallis whose group has published over 130 papers, and has interests in organic conductors, heterocyclic synthesis, anti-cancer agents as well as bond formation. The supervisory team includes Dr Chris Garner (organic chemistry) who has a wide experience of synthetic organic chemistry. The person undertaking this project will thus be exposed to different aspects of cutting edge organic chemistry in materials and medicinal chemistry which will strengthen his/her all round knowledge as preparation for the next career step. There is a 100% record of PhD completions in the group.

#### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **chemistry or related subject**.

Contact: [john.wallis@ntu.ac.uk](mailto:john.wallis@ntu.ac.uk) for informal discussions

## 27.

# ORGANIC CHEMISTRY: SYNTHESIS AND STRUCTURAL INVESTIGATION OF MOLECULES WITH PARTIAL BOND FORMATION

As two functional groups approach each other and undergo a chemical reaction there is a major reorganisation of the electron density in the region of these groups. Bond formation is of fundamental importance and underpins all reaction processes in chemistry and biology. A full understanding of how the bond forms can be achieved by structural measurements on a series of molecules which have these two groups in increasingly close proximity<sup>1-3</sup> and thus provide a series of “snapshots” of the reaction at different stages of separation between the reacting groups. The project will involve synthetic organic chemistry, some X-ray crystallography (which we can teach you) to measure how the two groups distort each other, as well as collaborations with two world class groups – one in solid-state NMR and the other in charge density measurements by X-ray diffraction to characterize the degree of bond formation between the functional groups.

This project will start by investigating models for two important reactions in organic chemistry: the attack of a phenol anion on a polarized alkene bond functionalized with electron-withdrawing substituents, and the attack of a boron-based electrophile on a more electron-rich alkene, with synthesis and study of molecules such as 1 and 2. The understanding of a reaction process is an area of international importance.

### References

- N. Mercadal, J.D. Wallis et al., *CrystEngComm*, 2014, 16, 8363; DOI: 10.1039/C4CE00981A
- A. Lari, J.D. Wallis et al., *Org. Biomolec. Chem.*, 2012, 10, 7763. DOI: 10.1039/C2OB25929J
- P.C. Bell, J.D. Wallis, *Chem. Commun.*, 1999, 256. DOI: 10.1039/A808488B
- F. Pop, J.D. Wallis, N. Avarvari et al., “Chirality Driven Metallic versus Semiconducting Behaviour in a Complete Series of Radical Cation Salts Based on Dimethyl-Ethylenedithio-Tetrathiafulvalene (DM-EDT-TTF)”, *J. Amer. Chem. Soc.*, 2013, 135, 17176-17186, DOI: 10.1021/ja408350r.
- E. Bresco, M. Pitak, S. J. Coles, M. Pilkington, J. D. Wallis, “The Use of the Triptycene Framework for Observing O---C=O Molecular Interactions”, *CrystEngComm.*, 2011, 13, 6978-6984; DOI: 10.1039/C1CE05955F; designated a “Hot Paper” by the journal.

**Supervisors:** Prof. John Wallis

### Supervisor biogs

The project will be led by Professor John D. Wallis whose group has published over 130 papers, and has interests in organic conductors, heterocyclic synthesis, anti-cancer agents as well as bond formation. The supervisory team includes Dr Chris Garner (organic chemistry) and there will be additional support from our collaborators on NMR and charge density. The person undertaking this project will thus be exposed to different aspects of cutting edge organic chemistry in materials and medicinal chemistry which will

strengthen his/her all round knowledge as preparation for the next career step. There is a 100% record of PhD completions in the group.

**Entry requirements**

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **chemistry, or related subject**.

Contact [john.wallis@ntu.ac.uk](mailto:john.wallis@ntu.ac.uk) for informal discussions.

## 28.

### C-H ACTIVATION METHODS FOR THE FUNCTIONALIZATION OF BIPYRIDINES

"C-H activation" is one of the most active new areas of organic chemistry for introducing new functionality into molecules.<sup>1</sup> The aim of this project is to develop such methods for the C-H functionalization of 2,2'-bipyridine (1) in the 3,3'-positions, to give substituted products 3; currently there is no good method for the synthesis of these valuable compounds, which have potential applications in coordination chemistry, metal-organic frameworks and catalysis.<sup>2</sup> By utilizing the nitrogen atom of one ring to direct the functionalization of the second ring, via organometallic intermediates such as 2,3 the project will target a range of catalytic bipyridine functionalizations including both C-C and C-heteroatom bond forming reactions.

#### References

- L. Ackermann, Chem. Rev. 2011, 111, 1315.
- J.D. Wallis et al., Eur. J. Inorg. Chem., 2002, 1889; K Liu et al, Cryst. Growth Design, 2014, 14, 6409.
- B. Butschke, H. Schwarz, Chem. Sci., 2012, 3, 308.

**Supervisors:** Dr. Warren Cross

#### Supervisor biogs

The project will be led by Dr Warren Cross, whose group concentrates on developing new C-H activation methods. The supervisory team includes Prof. John Wallis who has worked with 3,3'-bipyridines, and has interests in several aspects of heterocyclic synthesis. The person undertaking this project will gain experience in modern organometallic and organic chemistry.

#### Entry requirements

In order to be eligible to apply, you must hold, or expect to obtain, a UK Master's degree (or UK equivalent according to NARIC) with a minimum of a merit, and/or a UK 1st Class/2.1 Bachelor's degree (or UK equivalent according to NARIC) in **Chemistry or related discipline**.

**Contact:** [warren.cross@ntu.ac.uk](mailto:warren.cross@ntu.ac.uk) for informal discussions.