2018
School of science

HDR Research Projects

Applied Chemistry and Environmental Science

DR229/ MR229

Contents

Click on project links for more information

Dr Enrico Della Gaspera

- Novel p-type Transparent Conducting Oxides
- Plasmonic Semiconducting Nanocrystals: Bridging the Gap Between Metals and Semiconductors
- Photo-activity of Atomically Engineered Semiconductor Nanostructures

Dr Tamar Greaves

- Enzyme Biocatalysis in Ionic Liquids
- Interaction of novel cryoprotectants and model membranes

Dr Andrew Hung

- Conotoxins as Potential Novel Therapeutics for Neuropathic Pain
- Molecular mechanisms of action of dietary antioxidants and chromatinmodifying compounds

Dr Lathe Jones

- Applied Electrochemistry: New Nanostructured Materials for Energy Conversion Project name
- The Electrochemical Study of the Mineral Surfaces with Micron Resolution

Dr Ylias Sabri

- Design of Nanosized ceria-based Materials for Catalytic Oxidation Reactions Project name
- UV-assisted solid-state gas sensors for non-invasive diagnostic applications
- Colloidal lithography based nanostructures for numerous applications
- Building with smoke

Dr Sarvesh Soni

- Molecular biology meets Nanotechnology: An accurate, point-of-care diagnosis and bio-control for the pathogens causing Powdery Mildew and Botrytis in Grapes

Dr Nhiem Tran

- Self-assembled lipid nanoparticles for targeted cancer therapeutics
- Antimicrobial coating for orthopaedic implants
- Lyotropic liquid crystalline nanomaterials for encapsulation and delivery of siRNA

Dr Sylvia Urban

- Bioactivity assessment of natural products derived from Australian Terrestrial and Marine organisms and Exploration of Chemical Separation Methodologies
- Natural Product Studies of Australian Marine and Terrestrial Organisms – therapeutic potential
- Bioactivity guided evaluation of the chemical components of indigenous Australian plants and an assessment of their suitability as potential lead therapeutic compounds

Dr Joel van Embden

- Functional Nanocrystal Inks for Printed Inorganic Solar Cells
- Synthesis of Novel Semiconductor Materials for Thin Film Optoelectronics
- Solution-Processed Scalable Perovskite Solar Cells Using a Mini-Reactor

Chemistry of currently non-existent 2-Dimensional (2D) materials

Ian Potter NanoBioSensing Facility and NanoBiotechnology Research Laboratory - School of Science / Functional Materials and Microsystems Research Group [School of Engineering] – RMIT City

Project Description

This project is geared towards making new fundamental discoveries in the area of 2-Dimensional (2D) materials. The field of 2D materials is currently one of the most exciting avenues in materials research, and is already leading to the next wave of nanotechnology revolution. This is because 2D materials (extremely thin flakes similar to graphene but with other compositions) have started to show exotic properties that have been rarely encountered before. These include room temperature superconductivity, 2D electron gases, topological insulators, etc. The 2D materials may resemble graphene in morphology, but vary in compositing ranging from oxides to chalcogenides to elemental forms such as phosphorene, antimonene and silicene. Such new materials are interesting because they offer a finite bandgap which graphene lacks. Our group at RMIT has made recent breakthroughs in the synthesis of hitherto unknown 2D materials.

The PhD scholar will be involved in developing and understanding the chemistry of 2D materials. This will include (i) developing new chemical synthesis strategies to fabricate 2D materials, (ii) developing strategies to protect 2D materials from environmental oxidation, and (iii) functionalizing 2D materials with electron-donor, hole-donor and bio-molecules to tune their performance for a variety of applications. These applications will range from highly efficient electronics to energy generation to biosensing.

The PhD scholar will be based at the RMIT city campus and work collaboratively in a highly cross-disciplinary environment across the Schools of Science and Engineering at RMIT University. The project will involve a number of collaborations across several Australian Universities and research institutions across UK, Europe, Singapore and India. Facilities at Australian Synchrotron will be used to characterize these 2D materials. Other specialised techniques include microscopy (SEM, TEM, HRTEM); spectroscopy (absorbance, fluorescence, Raman, FTIR, EDX, EELS, XPS); crystallography (XRD); electrochemistry (voltammetry) and electronic measurements to understand fundamental properties. Materials with appropriate properties will then be used for relevant applications. This high-risk/ high-value project is ideally suited to somebody who is keen to make transformative discoveries in nanoscience.

References:

[1] Walia, S. & Bansal, V. et al., *2D Materials.* 4, 025110 (2017).
[2] Walia, S. & Bansal, V. et al., *2D Materials.* 4, 015025 (2017).
[3] Walia, S. & Bansal, V. et al., *Advanced Materials.* 29, 1700512 (2017).
[4] Walia, S. & Bansal, V. et al., *Nature npj 2D Materials & Applications.* 1, 18 (2017).

Contact Details:

To discuss this project further contact:
Professor Vipul Bansal (vipul.bansal@rmit.edu.au) Office +61 03 99252121
Dr Sumeet Walia (sumeet.walia@rmit.edu.au) Office +61 03 99252136

Broad light-responsive organic semiconductors for next-generation applications in catalysis, flexible electronics and wound healing

Applied Chemistry and Environmental Science Discipline/Ian Potter NanoBioSensing Facility and NanoBiotechnology Research Laboratory – RMIT City

Project Description

This Discovery project funded by the Australian Research Council will develop a new class of organic semiconductors that will show broad absorbance across the UV-Visible-IR light.[1,2] A library of hybrid inorganic-organic materials with new physico-chemical properties will be created by combining organic semiconductors with metals and metal oxides.

These nanomaterials will be grown on unique substrates such as textiles, hair, leaves and diatomaceous skeletons to develop next generation products that use light as a trigger to achieve functionality. The potential products include highly efficient photocatalysts for environmental remediation and energy production; flexible electronic devices for sensing and memory storage; and antibacterial agents for chronic wound healing.[3,4]

The PhD scholar will be based at the RMIT city campus and work collaboratively with Monash University and Australian Synchrotron. The project involves solution-based protocols to synthesize nanomaterials and use of specialised techniques including microscopy (SEM, TEM, HRTEM); spectroscopy (absorbance, fluorescence, FTIR, EDX, XPS); crystallography (XRD); electrochemistry (voltammetry) and electronic measurements to characterize the materials and obtain fundamental understanding of their properties. Materials with appropriate properties will then be used for relevant applications. Overall, this Discovery project will provide a highly cross-disciplinary training along with several high quality publications.

References:

[1] Nafady, A., O’Mullane, A.P. & Bond, A.M. *Coordin. Chem. Rev.* 268, 101-142 (2014).
[2] Mohammadtaheri, M., Ramanathan, R. & Bansal, V. *Catal. Today* 278, 319-329 (2016).
[3] Davoudi, Z.M., Kandjani, A.E., Bhatt, A.I., Kyratzis, I.L., O'Mullane, A.P. & Bansal, V. *Adv. Funct. Mater.* 24, 1047-1053 (2014).
[4] Pearson, A., Ramanathan, R., O'Mullane, A.P. & Bansal, V. *Adv. Funct. Mater.* 24, 7570-7579 (2014).

Contact Details:

To discuss this project further contact:
Professor Vipul Bansal (vipul.bansal@rmit.edu.au) Office +61 03 99252121
Dr Rajesh Ramanathan (rajesh.ramanathan@rmit.edu.au) Office +61 03 99252887

Color-based nano-sensors for establishing fingerprints of cancer cell

Applied Chemistry and Environmental Science Discipline/Ian Potter NanoBioSensing Facility and NanoBiotechnology Research Laboratory – RMIT City

Project Description

This project will develop new color-based biosensing tools for generating unique fingerprints of different types of cancer cells. This robust profiling of mammalian cells will aid in the detection of cancer at early stages of progression. To achieve this, the enzyme-like catalytic activity of the nanoparticles (NanoZyme) will be employed for the generation of colorimetric response.[1,2] These NanoZymes will be tagged with different molecular recognition elements such as DNA aptamers, carbohydrate binding lectins, and antibodies. A sensor array will then be created to obtain a fingerprint for each type of cell.[3] This tool is not only likely to aid in early detection of cancer but also developing personalized medicine, based on the unique biological profile of individual cancer patients.

The PhD scholar will (i) develop new chemical synthesis strategies to fabricate nanomaterials of controlled size and shape, (ii) assess the enzyme-like catalytic property to determine important kinetic parameters, (iii) combine the NanoZyme with molecular recognition elements to build sensor propers, (iv) create a sensor array to profile different cancer cells and (v) use advanced statistical tools to identify cancer cells in complex biological fluids.

The PhD scholar will be based at the RMIT city campus and work collaboratively in a highly cross-disciplinary environment at the Ian Potter NanoBioSensing Facility. The project will involve a number of collaborations across a number of Australian Institutes (Peter Macallum Cancer Institute, Deakin University) and research institutions across UK (University of Manchester) and USA (University of Massachusetts, Amherst). The PhD scholar will use specialized techniques including microscopy (SEM, TEM, HRTEM); spectroscopy (absorbance, fluorescence, FTIR, EDX, XPS); crystallography (XRD); biochemistry (confocal, FACS, ELISA) statistical analysis (cluster tools, discriminant tools, regression analysis) and color assessment for quantifying the sensor response using a simple mobile phone camera. Overall, this project will provide a highly cross-disciplinary training across materials science, nanotechnology, chemistry, cell biology and biochemistry along with high quality publications.

References:

[1] Weerathunge, P., Ramanathan, R., Shukla, R., Sharma, TK., & Bansal, V. *Anal. Chem.* 86, 11937-11941 (2014).
[2] Sharma, TK., Ramanathan R., Weerathunge, P., Mohammadtaheri, M., Daima, HK., Shukla, R., & Bansal, V. *Chem. Commun.* 50, 15856-15859 (2014).
[3] Wang, X., Hu, Y. & Wei, H. *Inorg. Chem. Front.* 3, 41-60 (2016)

Contact Details:

To discuss this project further contact:
Dr Rajesh Ramanathan (rajesh.ramanathan@rmit.edu.au) Office +61 03 99252887
Professor Vipul Bansal (vipul.bansal@rmit.edu.au) Office +61 03 99252121

NanoZyme sensors for color-based environmental, food and clinical analysis

Applied Chemistry and Environmental Science Discipline/Ian Potter NanoBioSensing Facility and NanoBiotechnology Research Laboratory – RMIT City

Project Description

This project will develop new color-based biosensing platforms for the rapid, easy-to-use detection of environmental pollutants, food contaminants and clinically relevant pathogens and molecules responsible for various diseases. The color generation in the presence of the target molecule will employ the enzyme-like catalytic activity of the nanoparticles (NanoZyme) while the ability to specifically detect the target analyte will be achieved by combining the NanoZymes with different aptamers (ssDNA).

The PhD scholar will be involved in (i) developing new chemical synthesis strategies to fabricate different nanomaterials with a control over their size, shape and compositions, (ii) using a number of high-end techniques to characterize the properties of nanoparticles, (iii) assess the enzyme-like catalytic property of nanomaterials to determine reaction kinetic parameters, (iv) combine the NanoZymes with aptamers through covalent and non-covalent interactions and (v) create biosensor and diagnostic platforms for the detection of environmental pollutants, food and clinically relevant pathogens.

The PhD scholar will be based at the RMIT city campus and work collaboratively in a highly cross-disciplinary environment. The project will involve a number of clinical partners across leading Australian research institutes (Burnet Institute, Peter Macallum Cancer Institute, Deakin University) and institutions across UK (University of Manchester), USA (University of Massachusetts, Amherst) and Spain (Universidad de Granada). The PhD scholar will use specialized techniques including microscopy (SEM, TEM, HRTEM); spectroscopy (absorbance, fluorescence, FTIR, EDX, XPS); crystallography (XRD); statistical analysis (cluster tools, discriminant tools, regression analysis) and color assessment for quantifying the sensor response using a simple mobile phone camera. Overall, this project will provide a highly cross-disciplinary training across materials science, nanotechnology, chemistry, cell biology and biochemistry along with several high quality publications.

References:

[1] Weerathunge, P., Ramanathan, R., Shukla, R., Sharma, TK., & Bansal, V. *Anal. Chem.* 86, 11937-11941 (2014).
[2] Sharma, TK., Ramanathan R., Weerathunge, P., Mohammadtaheri, M., Daima, HK., Shukla, R., & Bansal, V. *Chem. Commun.* 50, 15856-15859 (2014).
[3] Wei, H., Wang, E. *Chem. Soc. Rev*. 42, 6060-6093 (2013).

Contact Details:

To discuss this project further contact:
Professor Vipul Bansal (vipul.bansal@rmit.edu.au) Office +61 03 99252121
Dr Rajesh Ramanathan (rajesh.ramanathan@rmit.edu.au) Office +61 03 99252887

Protein Aerogels as Novel Bionanosensors

Applied Chemistry and Environmental Science Discipline – RMIT City

Project Description

This project will investigate and develop gold/silver-protein aerogels, a novel class of mesoporous biometallic composite materials. The Mezzenga group (ETH Zurich) recently reported these new aerogels formed by growing gold nanoparticles within a protein fibril matrix and then stabilized with supercritical carbon dioxide. These materials are, by weight, 98% air: 1.7% precious metal: 0.3% protein fibrils, and they have attracted international media interest. They are highly porous, homogeneous and tunable light-as-air nanomaterials with reported applications as catalysts and pressure sensors. Their composition and properties also make them potentially suitable as spectroscopic nanosensors.

In this project we will synthesise new aerogels, characterize their physical properties and structure, and explore their potential as a new class of biomaterial and nanosensor. In particular, we will tune their plasmon resonance responses to explore their ability to act as surface enhanced Raman spectroscopic (SERS) nanosensors. The project will also investigate aspects of molecular assembly and functionalization that will facilitate establishment of protocols for fabrication of the nanosensors. The project will be highly multidisciplinary, involving a combination of chemical, materials science and biological processes to synthesise different aerogels, with a range of advanced imaging and spectroscopic techniques being then used to investigate their structure and molecular organization.

This project will involve collaboration with the Mezzenga group at the ETH in Zurich, Switzerland, with expectation that the student will be willing to travel to our collaborator's lab for training.

References:

[1] Nystrom et al., Adv. Materials (2016) 28, 472–478, doi:10.1002/adma.201503465.
[2] Schluker, S., Angew Chem Int Ed Engl. (2014) 53, 4756-95.,doi: 10.1002/anie.201205748.

Contact Details:

To discuss this project further please contact:
Professor Ewan Blanch (ewan.blanch@rmit.edu.au) 1st Supervisor – Office 3.2.26
Professor Srinivasan Madapusi

Designing Photocatalysts for Gas Phase Reactions

Applied Chemistry and Environmental Science Discipline, Advanced Porous Materials Laboratory – RMIT City/CSIRO Manufacturing, Advanced Fibres & Chemical Industries, Clayton

Project Description:

In photocatalysis the absorption of light, generally by a semiconductor as the photocatalyst, initiates or accelerates a chemical reaction. This is due to photoexcitation, where an excited state is formed on absorbance of the photon energy. Separation of the electron and associated electron deficiency (hole) within the semiconductor results in redox reactions occurring with surface adsorbed species. Studies have shown that the composition and morphology of the photocatalyst are important parameters in determining how effective the photocatalyst is: For example, the composition can alter the range of wavelengths of light that the photocatalyst can absorb and the morphology can influence the number of surface active sites on which the reactions can occur.[1] Numerous studies exist on the application of such photocatalysts for the degradation of pollutants in water and air. Alternatively, rather than breaking down chemicals, photocatalysis can be used in organic synthesis.[2] In this project the focus will be on photocatalysed gas phase reactions.

The objectives of this research will be to design and synthesise photocatalytic materials to optimize light absorption and gas flow over the porous material. Following this, the photocatalyst will be tested for initiating or accelerating gas phase reactions that are of industrial importance. The student participating in this project will obtain training in chemical synthesis techniques, materials characterization (including electron microscopy, X-ray diffraction, gas sorption and thermogravimetric analysis), along with photocatalytic testing of the materials. The student will be expected to spend time in the laboratories of CSIRO Manufacturing in Clayton to conduct this project.

References:
[1]. H. Ren et al. J. Hazardous Mater. 2017, 325, 340-366. (Review)
[2]. X. Wu et al. J. Phys. D: Appl. Phys., 2017, 50 283001 (26pp). (Review)

Contact Details:
To discuss this project further please contact:
Prof. Rachel A. Caruso – Email: Rachel.caruso@rmit.edu.au Office 3.1.7C
Dr Xingdong Wang – Email: xingdong.wang@csiro.au

Photocatalysis Design and High-throughput Approaches to Testing for Application in Air Purification

Applied Chemistry and Environmental Science Discipline, Advanced Porous Materials Laboratory – RMIT City/CSIRO Manufacturing, Advanced Fibres & Chemical Industries, Clayton

Project Description:

Environmental pollution in both water and air results in adverse health effects. Air pollution consists of a variety of components of both particulate and gaseous nature. Photocatalysis is a promising, green approach to deal with gaseous air pollutants, specifically oxidation of volatile organic compounds and inorganic gases. The photocatalyst is generally a metal oxide semiconductor, usually a titania based material with a band gap energy of ~3.2 eV, which absorbs ultra-violet light. This generates electron-hole pairs that initiate the chemical reaction to break down the pollutants. Titania has the advantages of being readily available and inexpensive. However, it suffers from a relatively low photocatalytic activity caused by the recombination of photon induced electron and hole pairs and a wide band gap that requires high energy UV radiation (only 5% of sun light) to induce the reaction. Therefore, further modification of the existing TiO_2 materials is required to decrease the electron/hole recombination rate and decrease the band-gap of titania to allow photoactivity on irradiation with visible light.

Conventionally, significant time is required in the development of the photocatalyst; including material design, performance evaluation, and optimization. This PhD project will focus on developing and optimizing new photocatalytic materials and establishing processes for testing the efficiency of the materials for indoor and outdoor air purification under visible light using high-throughput approaches. High-throughput approaches allow multiple samples to be assessed simultaneously, significantly decreasing the time required for testing and therefore optimization of the photocatalyst.[2] To conduct this project, the student involved will learn a range of synthesis and characterization skills, including electron microscopy and X-ray diffraction analyses, as well as gas sorption studies, and will work with CSIRO to establish testing protocols and to test the effectiveness of the materials.

References:

[1]. H. J. Ren, P Koshy, W. F. Chen, S. H. Qi, C. C. Sorrell J. Hazardous Mater. 2017, 325, 340-366. (Review)
[2]. N. M. Nursam, X. D. Wang, R. A. Caruso ACS Combinatorial Sci. 2015, 17, 548-569. (Review)

Contact Details:

To discuss this project further please contact:
Prof. Rachel A. Caruso – email: rachel.caruso@rmit.edu.au Office: 3.1.7C
Dr Xingdong Wang – email: xingdong.wang@csiro.au

Smart Sensing of Toxins

Applied Chemistry and Environmental Science Discipline, Advanced Porous Materials Laboratory – RMIT City/CSIRO Manufacturing, Advanced Fibres & Chemical Industries, Clayton

Project Description

The ability to quickly and cheaply detect the presence of toxins in the environment is paramount for the conservation of our delicate ecosystems and for the prompt identification of sources that could compromise human health [1]; this issue can be addressed with highly sensitive, portable devices based on adaptive porous materials. The current technology requires sophisticated chemistry to determine the presence of toxins in samples which have to be collected, transported and then specifically prepared prior to analysis with expensive and complicated analytical equipment in specialised laboratories. The vision for this project is to build a portable platform for the immediate detection of toxins in the environment so that accurate, real-time monitoring can be performed (e.g. testing of storm water runoff to monitor for pollution).

Metal Organic Frameworks (MOFs) are a unique class of crystalline materials comprised of metal clusters linked together by rigid organic molecules, giving highly porous architectures with properties suitable for sensing, catalysis, filtration and bio-applications. MOFs have the ability to trap target molecules due to their tuneable pore sizes as well as signal the presence of these molecules through their intrinsic properties (i.e. luminescence). Significant technological progress is still required for the integration of MOFs into devices for the practical use of these exceptional materials [2, 3]. The current project will enable the fabrication of the next generation of sensors capable of working in real-time for high-throughput detection with unprecedented sensitivity.

The key to developing a successful sensor is to choose MOFs with the appropriate chemistry and porosity for selective uptake of the toxic molecules (heavy metals, carcinogens or volatile organic compounds). It is essential that the MOFs are water stable over a considerable amount of time under a range of conditions (pH, temperature, sunlight, etc.). The MOFs need to be placed on supports (e.g. polymers, metals, metal oxides) by various MOF patterning techniques [4]. The aim is to fabricate a working prototype device that can demonstrate the versatility and potential for these sensors. It is anticipated that future MOF sensors will not only have the capability to selectively detect toxins from contaminated air or water, but also the ability to signal the presence of these harmful molecules in real time so that their impact can be minimised.

References:

[1]. K. Austen, Nature, **517** (2015) 136.
[2]. C.M. Doherty et al., Acc. Chem. Res. **47** (2014) 396. (Review)
[3]. P. Falcaro et al., Chem. Soc. Rev. **43** (2014) 5513. (Review)
[4]. C.M. Doherty et al, Adv. Mater. **25** (2013) 4701.

Contact Details:

To discuss this project further please contact:
Rachel Caruso – Email: rachel.caruso@rmit.edu.au Office: 3.1.7C
Cara Doherty – Email: cara.doherty@csiro.au

Evaluating the environmental impact of sunscreens in Port Phillip Bay

Applied Chemistry and Environmental Science Discipline – RMIT City

Project Description

Australia has one of the highest rates of skin cancer in the developed world [1]. This has led to long-term use of public awareness campaigns and encouragement to 'slip, slap, slop' on sunscreens when outdoors. Most Victorians use sunscreen and frequently visit iconic beaches such as St Kilda and Middle Park. Although it is known that some sunscreen chemicals can affect microalgae [2], the effects of these chemicals on the marine environment have yet to be fully explored, and awareness of these effects is low among the general community.

Ultraviolet (UV) filters (UVF), UV light stabilizers (UVLS) and preservatives (PVS), are widely used worldwide in sunscreens and plastic commodities, which has resulted in their observation in rivers, lakes and coastal environments worldwide. In a recent pilot study, Assoc Prof Graeme Allinson examine the occurrence of common UVF and UVLS and preservatives in different estuaries in Port Philip Bay, Victoria, for the first time. In that context, 16 UVF and UVLS but only 5 of the screened preservatives were observed in water and/or sediment samples. The detection of common UV filters, such as 4MBC, OMC, OC and the common preservatives 2-PE, MP, and PB in these Victorian estuary proves that the existence of personal care products in the environment is not just an issue for more densely populated countries in the northern hemisphere, but also of concern in Australia.

In this project, seawater and sediment samples will be collected around highly populated beaches in Victoria and will be analysed for chemicals and nanoparticals (ZnO) used in sunscreens using gas chromatographic (GC-), liquid chromatographic (LC-), inductively coupled plasma (ICP-) mass spectrometric (MS) methods. The student will be trained to undertake chemical separation and concentration methods by Assoc. Prof Graeme Allinson; specific chemical analytical methods will developed in collaboration with Dr. Yutaka Kameda (Chiba University of Technology, Japan [2]) and applied by SEH technical staff to instruments in the chemical analytical facility at RMIT.

The data gathered will answer the following key question: are sunscreen chemicals found in sufficient quantities in Port Philip Bay to exert an effect on the local marine environment? There are no marine water quality guideline values for any of the UV filters sunscreens in Australia's current national water quality guidelines, so potential impact will be assessed by using risk quotients (RQ) and toxicity unit (TU) and concentration addition (CA) aquatic toxicity risk assessment methods.

There are no ethical concerns that need to be addressed or approvals that need to be obtained.

References:
[1]. Perez *et al.* (2015). Higher Education Research 30(2): 336-346.

[2]. Tashiro & Kameda (2013). Marine Pollution Bulletin 77: 333–340.

Contact Details:
To discuss this project further please contact:
Assoc Professor Graeme Allinson (Graeme.allinson@rmit.edu.au) – Office 3.2.23
Dr Sarvesh K Soni (sarvesh.soni@rmit.edu.au) – Office 223.1.06

Enhancing solar to chemical energy conversion with optical nanoantennas

Applied Chemistry and Environmental Science Discipline, *NanoSmart La, RMIT*

Project Description

Chemical reactions powered by light are used to generate increasingly complex organic molecules [1]. Unfortunately, the diffuse nature of sunlight is incompatible with the demands of many of the photo-catalysts utilized in these systems. Using a combination of cutting-edge experimental and theoretical approaches [2], the successful candidate will design, create and analyze hybrid metal/photo-catalyst nanostructures capable of improving photo-catalytic efficiencies under real-world conditions. Ultimately these improvements will be used to develop new applications towards the synthesis of high-value added fine chemicals.

In order to power chemical reactions, a photo-catalyst must first absorb sufficient light before converting this into chemical energy. One approach to improving efficiency is the enhancement of the catalyst's ability to absorb light via modification of its local density of states. It is possible to sculpt the electromagnetic density of states and achieve extremely high energy densities using metal nanoparticles that interact very strongly with light [3]. These strong interactions result from the excitation of *surface plasmons*: light-driven oscillations of electrons in the metal nanostructures. Under the right conditions these metal nanostructures act as optical antennae, collecting and channeling radiant energy to the photo-catalyst thus forming a transmitter-receiver pair [4]. This so-called "antenna effect" boosts the efficiency of not only light absorption, but a range of other physical phenomena (Raman scattering, triplet state formation, emission). Importantly, it can increase catalytic efficiency [5].

Hybrid photo-catalyst/nanoparticle structures will be prepared by a combination of clean-room and wet-chemical synthesis techniques. The structural properties of the absorbers will be characterized using a suite of techniques, such as electron microscopy (SEM & TEM), X-ray diffraction and atomic force microscopy. The optical properties will be characterized by means of micro-spectrometry in the visible and near-infrared. Importantly, the application of the developed structures as catalysts in the synthesis of complex organic molecules will be assessed using reaction-discovery principles. Techniques such as multinuclear NMR, mass spectrometry, chromatography and other spectroscopic capabilities are important for this projects. The expected outcome of this project, funded by an ARC Future Fellowship, is a detailed understanding of the interplay between discrete molecule photo-catalysts and metal nanoparticle optical antennas and the result of this on photo-catalytic organic synthesis.

References:

[1]. D. M. Schultz and T. P. Yoon, Science 343, 1239176 (2014)
[2]. T. U. Connell, S. K. Earl, C. Ng, A. Roberts, T. J. Davis, J. M. White, A. Polyzos and D. E. Gómez, Small, 10.1002/smll.201700692 (2017)
[3] M. Xiao, R. Jiang, F. Wang, C. Fang, J. Wang, J. C. Yu, J. Mater. Chem. A 1, 5790 (2013)
[4] J. C. Scaiano, K. Stamplecoskie, J. Phys. Chem. Lett. 4, 1177 (2013)
[5] K. Mori, M. Kawashima, M. Che, H. Yamashita, Angew. Chem., Int. Ed. 49, 8598 (2010)

Contact Details:

To discuss this project further please contact:

Associate Professor Daniel Gomez (daniel.gomez@rmit.edu.au) Bld 3.1.2A
Dr. Timothy Connell (tim.connell@rmit.edu.au)

Plasmon- Exciton Polaritons: Hybrid light-matter states

Chemistry and Physics, *NanoSmart Lab* and The Centre of Excellence in Exciton Science RMIT City Campus

Project Description

Harvesting solar energy can provide a significant fraction of the world's energy need over the next century. When solar radiation interacts with matter, *excitons* (electronic excitations) are created and their dissociation can result in the production of an electrical current (the working principle of solar cells). Conversely, excitons can also be created when an electric current flows through a material, and subsequently recombine to produce light (the reverse of a solar cell), the basis for creating displays and LEDs.

A fundamental problem with technologies based on excitons is that most molecular materials interact very weakly with light. An approach to overcome this limitation consists on creating hybrid metal-molecule nanostructures. Metal nanostructures are a class of materials capable of interacting very strongly with light, as a result of the excitation of *surface plasmons*: light-driven oscillations of electrons in the metal nanostructures [1].

The resonance coupling between a plasmonic nanostructure and an exciton occurs when their electronic excitation energies are strongly overlapped [1-3]. With a good match of the energy levels, and close enough molecule–nanostructure separations, the orbitals of the two constituents can be efficiently *hybridized* to create new resonant states called *plasmon-exciton polaritons* [1,3]. Under this interaction regime, many molecular and material properties are severely affected, including increased: electrical conductivity [2], chemical reactivity [4] and metal-to-semiconductor electron transfer [5].

The aim of this project is to create novel metal-molecule structures exhibiting strong plasmon-exciton interactions, and study the effect of these interactions in charge separation processes for applications in solar energy harvesting and conversion, with an emphasis in photo-chemistry. The hybrid materials will be prepared by a combination of clean-room and chemical synthesis techniques. The structural properties will be characterized using a suite of techniques, such as electron microscopy (SEM & TEM), X-ray diffraction and atomic force microscopy. The optical properties will be characterized by means of micro-spectrometry in the visible and near-infrared. This project is partly funded by an ARC Future Fellowship and the Centre of Excellence in Exciton Science, with whom the student will have access to state-of-the-art theoretical and experimental tools for understanding plasmon-exciton interactions.

References:

[1] P. Törmä and W. L. Barnes *Reports on Progress in Physics* **78**, 013901 (2015)
[2] T. W. Ebbesen *Accounts of Chemical Research* **49**, 2403(2016)
[3] D. E. Gomez, K. C. Vernon, P. Mulvaney, and T. J. Davis *Nano Letters* **10**, 274 (2010)
[4] C. Ng, S. Dligatch, H. Amekura, T. J. Davis, and D. E. Gómez *Advanced Optical Materials* **3**, 1582 (2015)
[5] P. Zeng, J. Cadusch, D. Chakraborty, T. A. Smith, A. Roberts, J. Sader, T. Davis, and D. E. Gomez *Nano Letters* **16**, 2651 (2016)

Contact Details:

To discuss this project further please contact:
Associate Professor Daniel Gomez (daniel.gomez@rmit.edu.au) Bld 3.1.2A
Professor Salvy Russo (salvy.russo@rmit.edu.au)

Solar to chemical energy conversion with plasmonic super-absorbers of light

Applied Chemistry and Environmental Science Discipline, *NanoSmart Lab* - RMIT

Project Description

Imagine a future chemical industry where chemical reactions are powered directly by sunlight! [1]. Using a combination of cutting-edge experimental [2] and theoretical approaches [3], the successful candidate will create nanostructures that are capable of absorbing nearly all incident visible light (super-absorbers), study their optical properties, and develop applications of these materials for the synthesis of high-value added fine chemicals.

Super-absorbers of light [2,4] are a class of materials that exploit the concept of optical impedance matching and ideally absorb all incident radiation, irrespective of its wavelength and angle of incidence. The absorbed energy is typically converted to heat, but under specific conditions, the energy can also be transformed into other more ‘useful’ forms for applications in photovoltaics, biological sensing, photo-detectors and also in photochemistry: the conversion of radiant energy into chemical potential energy.

One approach to realize these materials focuses on using metal nanostructures capable of interacting very strongly with light [2-4]. These strong interactions result from the excitation of *surface plasmons*: light-driven oscillations of electrons in the metal nanostructures. These plasmons can result in the emission of energetic (hot) electrons [5], which may be harvested for driving chemical reduction and oxidation reactions. This results in a net transduction of solar-to-chemical energy. The overall process is initiated by the absorption of light and, consequently, it is anticipated that *plasmonic super-absorbers* will be a class of highly efficient converters.

The plasmonic super-absorbers will be prepared by a combination of clean-room and chemical synthesis techniques. The structural properties of the absorbers will be characterized using a suite of techniques, such as electron microscopy (SEM & TEM), X-ray diffraction and atomic force microscopy. The optical properties will be characterized by means of micro-spectrometry in the visible and near-infrared. Importantly, the application of the developed super-absorbers in photo-chemistry will be assessed by means of organic reaction discovery, for which techniques such as NMR, chromatography and other spectroscopic capabilities are important. The expected outcome of this project, funded by an ARC Future Fellowship, is a detailed mechanistic understanding of the role of nanoparticle size, geometry and composition on their optical and photochemical properties.

References:

[1]. D. M. Schultz and T. P. Yoon, Science **343**, 1239176 (2014)
[2]. C. Ng, J. Cadusch, S. Dligatch, A. Roberts, T. J. Davis, P. Mulvaney, and D. E. Gomez, ACS Nano **10**, 4704 (2016).
[3] T. J. Davis and D. E. Gomez, Reviews of Modern Physics **89**, 011003 (2017)
[4] C. Ng, L. W. Yap, A. R. W. Cheng, and D. E. Gomez, Adv. Funct. Mater **27**, 10.1002/adfm.201604080 (2016)
[5]. M. L. Brongersma, N. J. Halas, and P. Nordlander Nature Nanotechnology **10**, 25 (2015)

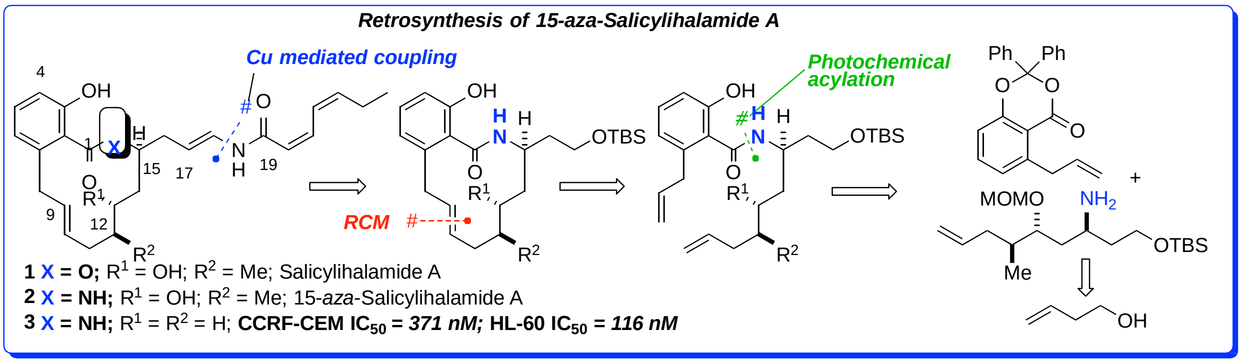
Contact Details: To discuss this project further please contact:
Associate Professor Daniel Gomez (daniel.gomez@rmit.edu.au) Bld 3.1.2A
Dr Timothy Connell (tim.connell@rmit.edu.au)

Total Synthesis of Aza Analogue of Myxobacteria Metabolite: 15-Aza- Salicylihalamide A (2) and related compounds

Chemistry and Environmental Science Discipline/Synthesis Research Group – RMIT City

Project Description

Myxobacteria are a life form at the interface between single and multicellular organisms. It is particularly remarkable that myxobacteria specialize in the production of compounds with mechanisms of action that are rare such as electron transport inhibition.[1] Extracts of several *Chondromyces* species showed high cytotoxicity against cultivated mammalian cells and bioassay-guided fractionation of extracts of a variety of strains including *Chondromyces apicularus* and *robustus* revealed the cytotoxicity was due to novel macrolides including *salicylihalamide A (**1**).*



Key to its success as a cancer therapeutic agent is the fact that the transformation to a lactam linkage makes it less susceptible to hydrolytic cleavage *in vivo* than the lactone in the natural product whilst the overall conformation and electronic properties of the lactam analogue remain similar. Nitrogen or aza modified derivatives of macrolide natural products are important clinically relevant compounds predominantly used for the treatment of human bacterial infections and various types of cancer.[2]

A retrosynthetic analysis of 15-aza-salicylihalamide A (2) is shown above. We have recently reported the synthesis of the simplified 15-*aza*-salicylihalamide A analogue (**3**) showed potent activity against several leukemia cell lines and was comparable to the activity profile of bafilomycin but 10 times less active on average.[3] The majority of SAR studies have been conducted on derivatives with modified enamide side chains and it has been shown that the presence of some form of enamide functionality is critical for activity.[4]

This chemical synthesis project involves the preparation of 15-*aza*-salicylihalamide A (**2**) and related novel derivatives. The biological testing of all products will be performed by our collaborators at WEHI. It is anticipated that this research will deliver new efficient and scalable chemical technologies for the production of biologically active compounds. The promising and very potent bioactivities of myxobacteria metabolites, their natural scarcity, structural uniqueness, coupled with our passionate interest to make them available by chemical synthesis for extensive analysis and better understanding of their molecular activity mechanisms, is our major research focus.

References:

[1]. Reichenbach, H. *J. Ind. Microbiol. Biotechnol.* **2001**, *27*, 149.
[2]. Hügel, H. M.; Smith, A. T.; Rizzacasa, M. A. *Org. Biomol. Chem.* **2016**, *14*,11301. [3]. Balan, D. *et al. Org. & Biomol. Chem.* **2012**, *10*, 8147.
[4]. Palimkar, S. S.; Uenishi, J.; Ii, H. *J. Org. Chem.* **2012**, *77*, 388. Nicolaou, K.; Kim, D.; Baati, R. *Chem. Eur. J.* **2003**, *9*, 6177.

To discuss this project further please contact:

A/Prof Helmut Hügel (helmut.hugel@rmit.edu.au) 1st Supervisor – RMIT city campus 3.3.9
Mr Trevor Rook (trevor.rook@rmit.edu.au) 2nd Supervisor – RMIT city campus 3.2.22

DR229 – PhD (Applied Chemistry)
MR229 – Master of Science (Applied Chemistry)

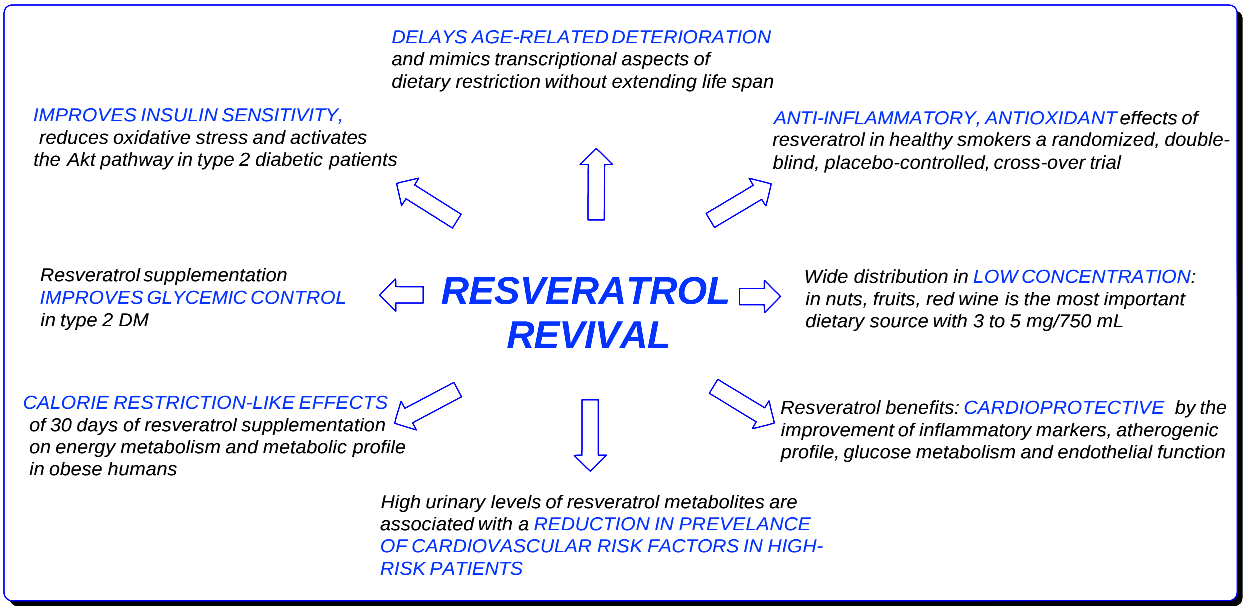
School of Science HDR Project 2018

Synthesis & Analysis of Resveratrol Related Beverages, Foods

Chemistry and Environmental Science Discipline/Synthesis Research Group RMIT- City Campus

Project Description

Dementia is a growing global challenge and a huge human burden. Around 47 million people worldwide were estimated to be living with dementia in 2015, and by 2030, the number of people with Alzheimer's disease is expected to rise to more than 70 million. Diet is considered to be the most significant common epidemiological contributing factor to health and overall well- being. *Constructing beverages, foods from a* class of molecules that treats multiple age-related diseases and dementia would have a major impact on global healthy aging and economics, generate *global health connections for people and reward consumers.* The Figure below highlights some of resveratrol's potential beneficial uses, including cardio-protective, neuro- protective, anti-inflammatory activity and in cancer chemo-protection. Whilst its low potency and multiple actions appear to limit its medicinal applications, the regular consumption of resveratrol-beverages and foods therefore might prove to be advantageous and therapeutically useful. The research strategy is to discover cost-effective synthesis of resveratrol and related polyphenols that can be used to prepare beverages and foods.



The project plan is to generate scalable green chemical syntheses of resveratrol and other stilbene polyphenols and produce beverages/foods, such as *Rescafe, Resveratea, Reschocolate*, and others in collaboration with RMIT Biosciences and Food Technology.

References:

[1]. Hügel, H.M. Brain food for AD-free ageing: focus on herbal medicines. Natural compounds as therapeutic agents for amyloidogenic disease. *Adv. Exper. Med. Biol.* **2015**, *863*, 95. [2]. Keylor, M. H.; Matsuura, B. S.; Stephenson, C. R. J. Chemistry and biology of resveratrol- derived natural products. *Chem. Rev. 2015*, 115, 8976 [3]. Hügel, Helmut M.; Jackson, N.; May, B.; Zhang, A.L.; Xue, C.C. Polyphenol Protection and Treatment of Hypertension. *Phytomed.* **2016**, *23*, 220. [4]. Baur, J. A. *et al.* Resveratrol improves health and survival of mice on a high-calorie diet. *Nature*, 2006, 444, 337.

Contact Details:

A/Prof Helmut Hügel (helmut.hugel@rmit.edu.au) 1st Supervisor – RMIT City campus 3.3.9
Dr Tien Hunyh (tien.hunyh@rmit.edu.au) 2nd Supervisor – RMIT Bundoora 223.1.68

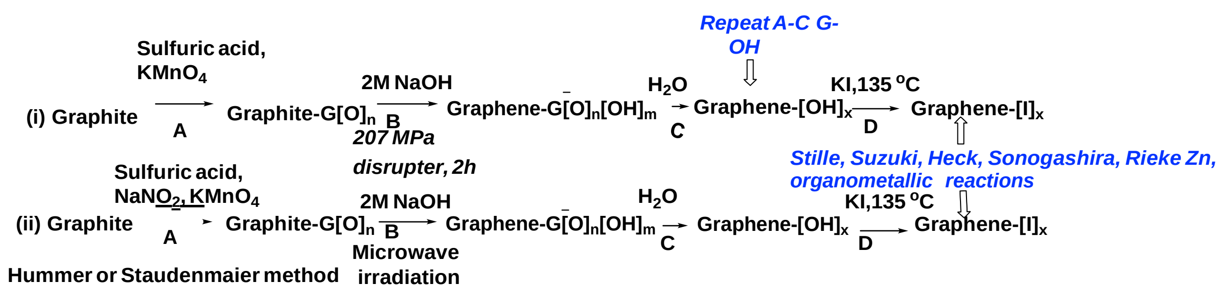
Tuning graphite into polyphenolic-multifunctional platforms for versatile biographene applications

Chemistry and Environmental Science Discipline/Synthesis Research Group – RMIT City

Project Description

Graphene is a 2D planar material consisting of sp^2 -hybridized carbon atoms organized in a hexagonal lattice and predominantly characterized by high electron mobility and mechanical flexibility and robustness.[1] Single layered graphene oxide has many applications of potential promise. For example, the synthesis of multifunctional hexagonal carbon frameworks for exploration of interactions with nerve-cell signalling has huge technology potential to discover the molecular basis of memory. Also graphene adhesion to cell membranes may uncover the exocytic and endocytic trafficking systems, that are important for physiological synaptic
transmission. With this background and biological-graphene application focus, it is necessary to discover/synthesise versatile biocompatible graphene-platforms.
Therefore, the research aim is to generate tuneable multifunctional graphite platforms. The preliminary chemical transformations will be demonstrated by multiple synthesis functional group inter-conversions of gallic acid into products composed of lipophilic and hydrophilic pendant groups. This will then lead to polyhydroxy-graphite-graphene[2] and to further functional transformations[3,4] depicted below.

Tuning graphite to polyphenolic-multifunctional platforms for versatile biographene applications



The physical chemistry, physics and physiology of this one-atom-thick hexagonal carbon framework uniquely combines extreme mechanical strength, exceptionally high electronic and thermal conductivities, impermeable to gases, as well as many other supreme properties, all of which make it highly attractive for numerous biochemical and chemical applications and transformations, some of which will be investigated in this project.

References:

[1]. Novoselov K.S. *et al. Nature*, **2012**, *490*, 192.
[2]. Sun J. *et al. ACS Appl. Mater. Interfaces*, **2016**, *8*, 10226.
[3]. Katayama T. *et al. J Am. Chem. Soc.* **2016**, *138*, 5210.
[4]. Luo J. *et al. ACS Sustainable Chem. Eng.*, **2016**, *4*, 1404.

Contact Details:

To discuss this project further please contact:
A/Prof Helmut Hügel (helmut.hugel@rmit.edu.au) 1st Supervisor – RMIT city campus 3.3.9
Mr Trevor Rook (trevor.rook@rmit.edu.au) 2nd Supervisor – RMIT city campus 3.2.22

Quantum Mechanical Modelling of Silicene Supported on Silver and its Reaction with Atmospheric Gases

Applied Chemistry and Environmental Science Discipline/Computational Materials Chemistry Group/Raman Spectroscopy Group) – RMIT City

Project Description

This project will involve quantum mechanical modeling of two-dimensional silicene-based films. Two-dimensional (2D) nanomaterials have become one of the most quickly growing areas in science due to their unique properties and ability to form layers in various electronic devices. Silicene, composed solely of Si atoms arranged in a hexagonal honeycomb network [1], is one of the most promising 2D-nanomaterials as it is highly compatible with existing electronic devices. Its widespread application is, however, currently hindered by its instability in air.

Silicene has been grown under ultra-high vacuum conditions via evaporative deposition on a number of substrates, but primarily on the Ag(111) surface. When this system is exposed to oxygen, the silicene layer is readily oxidized and can delaminate from the underlying substrate at low or high oxygen doses [2,3]. The extent of oxidation, however, can alter the electronic properties and hence control of the process is highly desirable so as to obtain non-oxidized, partially-oxidized, or fully-oxidized silicene. Recent work has shown that by placing silicene between planar crystals of calcium fluoride and calcium disilicide, it is possible to obtain a wavy bilayer form of silicene that is highly resistant to oxidation [4]. Further work is required in order to determine how the supported silicene reacts with other gases present in the atmosphere and also ways to protect the silicene.

The aim of this project is to use density functional theory calculations and *ab initio* molecular dynamics simulations to determine how different gases react with the surface supported silicene and the associated electronic, structural and spectroscopic properties. Functionalisation of the supported silicene layer with different chemical groups will also be modeled in order to determine the electronic properties and how resistant is the material to reaction with oxygen and other gases. The calculations will be performed using several high performance supercomputing facilities within Australia. The findings from this work will be beneficial to the current drive for fabrication of smaller and thinner electronic devices, batteries and gas sensors.

References:

[1] M.J.S. Spencer (Ed), T. Morishita (Ed), Silicene: Structure, properties and applications, Springer (2016) ISBN 978-3-319-28342-5. (Review)
[2] T. Morishita, M.J.S. Spencer, Scientific Reports 5 (2015) 1750.
[3] X. Xu, J. Zhuang, Yi Du, H. Feng, N. Zhang, C. Liu, T. Lei, Jiaou Wang, M. Spencer, T. Morishita, X. Wang, S. Xue Dou, Scientific Reports 4 (2014) 7543.
[4] R. Yaokawa, T. Ohsuna, T. Morishita, Y. Hayasaka, M.J.S. Spencer, H. Nakano, Nature Communications 7 (2016) 10657.

Contact Details:

To discuss this project further please contact:

A/Prof. Michelle Spencer (michelle.spencer@rmit.edu.au) Senior Supervisor – Office 3.2.15
Prof. Ewan Blanch (ewan.blanch@rmit.edu.au) Associate Supervisor – Office 3.2.26

Solid Electrolyte Interphase Formation Mechanisms and Lithium Battery Design

Applied Chemistry and Environmental Science Discipline/ Computational Materials Chemistry Group) (City)/ Advanced Manufacturing and Fabrication (Manufacturing, Mechatronics and Materials: Rapid Materials Discovery and Fabrication Group RMIT City / CSIRO (Clayton)

Project Description

This project will involve modeling and characterisation of the reactions that occur on the surface of lithium-based battery electrodes.

Lithium metal has the highest specific energy (3800 $mAh.g^{-1}$) of all electrode materials that can be used in a lithium-type battery. It is the key to the next generation batteries such as lithium– sulfur and lithium-air [1]. However, the highly reactive nature of lithium, especially to electrolytes based on carbonate solvents, makes this electrode extremely challenging for use in real devices [1]. Typically, the cycle life of batteries using lithium metal is extremely low, due to the inability to plate lithium metal in two-dimensions during charging. Those materials that can support two-dimensional charging such as ionic liquids are limited to low current densities to preclude the formation of dendritic structures that can penetrate separators and contact the cathode material [2].

One of the “barriers” to dendritic growth of lithium is the presence of a stable solid electrolyte interphase (SEI): an interphase that consists of decomposition products of the electrolyte that form on the surface of lithium metal. Typically, it is highly conductive to lithium ions but insulating to electrons. It should remain relatively thin such that its contribution to the ohmic resistance of the device does not lead to self-discharge. By understanding how the SEI is formed via the decomposition of electrolyte products, we should be able to “reverse-engineer” the design of electrolytes for lithium metal batteries.

This work seeks to better understand how ionic liquid cations and anions decompose on the surface of lithium metal to form the SEI using quantum mechanical modeling methods. To complement these theoretical studies, FTIR, Raman, X-ray photoelectron spectroscopy (XPS), and electrochemical techniques will be used to evaluate the interface between lithium metal and these electrolytes. Overall the project will determine how molecular surface binding is able to control electrochemical activity.

References:

[1] J-G. Zhang, W. Xu, W.A. Henderson, Lithium Metal Anodes and Rechargeable Lithium Metal Batteries, Springer (2017) ISBN 978-3-319-44054-5. (review)
[2] M.D. Brennan, M. Breedon, A.S. Best, T. Morishita, M.J.S. Spencer, Electrochim. Acta, 243 (2017) 320.
[3] A. Basile, A.I. Bhatt, A.P. O'Mullane, Nat. Commun 7 (2016) 11794.

Contact Details:

To discuss this project further please contact:
A/Prof. Michelle Spencer (michelle.spencer@rmit.edu.au) Senior Supervisor – Office 3.2.15
Prof. Ivan Cole (ivan.cole@rmit.edu.au) Associate Supervisor – Office 57.3.12A

Designing Next Generation Robust Hybrid Porous Materials for Detecting and Capturing Harmful Pollutants.

Applied Chemistry and Environmental Science Discipline – RMIT City / Applied Porous Materials Team (CSIRO)

Project Description

An exciting opportunity is available for an outstanding PhD candidate to work on an ARC funded project on computational design of next generation hybrid porous materials for detecting and capturing harmful pollutants that are carcinogenic and degrade environmental quality. The past decade has seen the emergence of metal organic frameworks (MOFs) or porous coordination polymers (PCPs) as potential candidate materials across a plethora of applications [1, 2]. MOFs are crystalline materials built from metal ions or clusters bridged by organic linkers to form one-, two- or three-dimensional structures. ***MOFs are porous materials that hold the world record for specific surface area and storage of gases.*** MOF research has become one of the fastest growing fields in materials science. More than 20,000 different MOFs have been reported and studied within the past decade and nearly 130,000 hypothetical MOFs have been designed based on different metal clusters and ligands [2]. However, their uptake by industry is hamstrung by a lack of knowledge of their *in situ* performance under realistic conditions and the stability of MOFs in different thermal, chemical and mechanical environments [3]. Understanding these issues is critical for MOF manufacturing, processing and performance. This project will focus on fundamental understanding of what makes MOFs stable in realistic conditions using state of the art computational techniques [4] and to exploit this new understanding to guide development of robust porous materials for capturing harmful pollutants. We seek chemistry/physics/engineering graduates who have some background in any of the following: atomistic modelling, *in silico* design of materials, programming, high-throughput screening, Monte Carlo methods and first principles calculations.

The project involves close collaboration with experimentalist in the field of nanomaterials and device fabrication. Specifically, the project involves: (i) Develop *in silico* screening tool for pre-screening thousands of materials for capturing harmful pollutants. (ii) Develop new descriptors based on the structure–property relationship to identify materials that merit experimental characterisation. (iii) Use a combinatorial approach integrating modelling and chemical experiments to speed up the design cycle from laboratory testing to industrial use. (iv) Develop understanding of the stability of MOF materials in realistic conditions to find the best, robust materials for large-scale synthesis.

References:

[1]. J. Jiang *et al.* Chemical Society Reviews **40** (2011) 3599.
[2] M. Rubio-Martinez *et al*. Chemical Society Reviews **46** (2017) 3453.
[2]. C. E. Wilmer *et al*. Nature Chemistry 4 (2012) 83.
[3]. A. J. Howarth *et al*. Nature Reviews, Materials 1 (2016).
[4]. J. D. Evans *et al*. Chemistry of Materials 29 (2017) 199.

Contact Details:

To discuss this project further please contact:

Dr Ravichandar Babarao (ravichandar.babarao@rmit.edu.au) – Office 3.1.02A
Dr Xavier Mulet (Xavier.mulet@csiro.au) – New Horizon Building, Clayton

Novel *p*-type Transparent Conducting Oxides

Applied Chemistry and Environmental Science Discipline/NanoChemistry Laboratory – RMIT City

Project Description

This project aims to develop novel *p*-type metal oxides in order to achieve materials transparent in the visible wavelengths, and with enhanced electrical properties. While current transparent conducting oxides (TCOs) are based on *n*-type semiconductors, these novel *p*-type TCOs will enable the fabrication of highly efficient all-oxide electronic devices.

Specifically, this proposal focuses on delafossite-type materials, because they represent one of the most promising classes of materials for application in *p*-type transparent conductors. Delafossite oxides are in the form ABO_2 where *A* is a monovalent ion (usually copper) and *B* is a trivalent ion such as aluminum or gallium. Although these oxides have been studied for several years [1], at present there are no available recipes for the synthesis of high quality delafossite oxide nanoparticles. Moreover, the doping of such materials has been hardly investigated.

The first part of this project involves the development of a synthesis protocol for delafossite oxide nanoparticles. Once the synthesis is established, the *p*-type character of the material will be enhanced with doping strategies, through the substitution of the trivalent cation with divalent ions such as zinc and magnesium [2]. This strategy is inspired by that adopted for enhancing the properties of traditional *n*-type TCOs [3]. These materials will be used to fabricate thin films of optical/electronic quality, specifically targeting scalable, large area deposition methods such as spray coating. Moreover, to further improve the conductivity of the deposited coatings, various post-deposition strategies will be developed, including the use of molecular "solders" [4]. These materials will then be used within thin film devices, especially all-oxide electronics.

This multidisciplinary project supports a research initiative funded by the Australian Research Council (ARC) and bridges chemistry, physics and nanotechnology. The candidate will learn materials chemistry and thin-film fabrication protocols, and become skilled in characterisation techniques including x-ray diffraction, various spectroscopies (UV-Vis, PL, ellipsometry, Raman, XPS) and microscopies (SEM, TEM, AFM). Moreover, it will enable the candidate to develop valuable skills not only in the field of nanotechnology, but useful also for future career opportunities, including academia, consulting, and manufacturing and chemical industries.

References:

[1]. Z. Wang *et al*. Advanced Materials, **28** (2016) 3831. (Review)
[2]. T. S. Tripathi *et al.* Advanced Electronic Materials, **3** (2017) 1600341.
[3]. E. Della Gaspera *et al*. Journal of the American Chemical Society, **135** (2013) 3439.
[4]. D. Dolzhnikov *et al*. Science, **347** (2015) 425.

Contact Details:

To discuss this project further please contact:

Dr. Enrico Della Gaspera (enrico.dellagaspera@rmit.edu.au) 1st Supervisor – Office 3.2.7

Plasmonic Semiconducting Nanocrystals: Bridging the Gap Between Metals and Semiconductors

Applied Chemistry and Environmental Science Discipline/NanoChemistry Laboratory – RMIT City

Project Description

Plasmonic semiconductors have recently emerged as attractive materials for several applications including transparent electrodes, chemical probes, infrared light concentrators and smart windows. They have the potential to bridge the optoelectronic gap between traditional semiconductors and metals, combining visible transparency, distinctive absorptions in the near infrared and high electrical conductivity [1,2]. This project specifically targets zinc oxide (ZnO) as candidate for transparent electrode and infrared plasmonic applications. Although ZnO has been extensively studied for such applications, its properties are still inferior compared to other plasmonic semiconductors that contain expensive or toxic elements (such indium or cadmium oxides) or have environmental stability issues (copper chalcogenides) [3].

This project aims to develop recipes for doped ZnO nanocrystals with enhanced optical and electrical properties which are also highly tunable. This will be achieved by combining doping with trivalent and tetravalent cations, codoping with halides and hydrogen, promoting the formation of oxygen vacancies and tailoring the distribution of dopants within the nanocrystals [3,5]. The main challenge is to find balance between the amount of charge carriers provided by doping that triggers the insulator-to-metal transition, and the structural/electronic defects that are generated [2]. The ability to achieve atomically designed nanoparticles, and to process them into nanocrystalline coatings will enable vital advancements in the fields of optics and electronics. Moreover, the dopant-induced surface plasmon resonance in the near infrared makes these doped semiconductors extremely interesting also for applications in catalysis and sensing.

This highly multidisciplinary project is partially funded by the Australian Research Council (ARC) and will involve skills in nanomaterials synthesis, advanced characterisation and device fabrication. The candidate will gain expertise in high resolution TEM and related techniques (EDS, EELS), several spectroscopies (visible, infrared, Raman, and x-ray/UV photoemission spectroscopies) and various electrical measurements. The skills developed during the PhD will be highly valuable for several career opportunities both within and outside academic research.

References:

[1]. A. Comin and L. Manna, Chemical Society Reviews, **43** (2014) 3957. (Review)
[2]. T. Chen *et al*. Nature Materials, **15** (2016) 299.
[3]. I. Kriegel *et al*. Physics Reports, **674** (2017) 1. (Review)
[4]. E. Della Gaspera *et al*. ACS Nano **8** (2014) 9154.
[5]. X. Ye *et al*. Journal of the American Chemical Society, **138** (2016) 9316.

Contact Details:

To discuss this project further please contact:
Dr. Enrico Della Gaspera (enrico.dellagaspera@rmit.edu.au) 1st Supervisor – Office 3.2.7

Photo-activity of Atomically Engineered Semiconductor Nanostructures

Applied Chemistry and Environmental Science Discipline/NanoChemistry Laboratory – RMIT City

Project Description

The interaction between materials and light is at the core of many technological applications such as solar cells, clean fuel generation (water splitting), photocatalysis, and optical gas sensors. In order for a material to successfully absorb and utilize the energy provided by light, its physical, chemical and electronic properties have to be carefully designed and optimised.

The aim of this project is to fabricate light-absorbing coatings for a variety of applications such as catalysis, energy generation and sensing. In details, two deposition techniques will be used, Chemical Bath Deposition (CBD) and Successive Ionic Layer Adsorption and Reaction (SILAR) [1,2]. Both these techniques enable the deposition of semiconductors in the form of crystalline nanomaterials on desired surfaces such as glass, metal or plastic. The candidate will explore the parameter space of both CBD and SILAR reactions for the deposition of nanomaterials including zinc oxide, bismuth sulfide, and ternary compounds such as vanadates and oxynitrides. These materials are of great technological and industrial interest for use in optoelectronics, catalysis and energy generation, thanks to their selective light absorption properties [3,5]. The prepared coatings will be fully characterised combining both conventional and innovative techniques, including a custom-designed photoelectrochemistry platform. Importantly, compared to other deposition methods, CBD and SILAR require lower temperatures (below 100 °C), can be conducted on large, non-planar support surfaces, and are environmentally friendly (the solvent used is mainly water). These are all major advantages that will ultimately enable the translation of small scale devices into proof-of-concept, large area devices, validating the potential use of these materials within a broader industrial/commercial landscape.

This highly multidisciplinary project is embedded within a broader research initiative partially funded by the Australian Research Council (ARC), and involves collaborations with both local (CSIRO) and international institutions (University of Padova, Italy). The candidate will develop a deep understanding in the chemistry and physics of nanomaterials and related devices, learn advanced characterisation techniques and gain invaluable skills for their future career.

References:
[1]. G. Hodes, Physical Chemistry Chemical Physics, **9** (2007) 2181. (Review)
[2]. H. J. Lee *et al*. Nano Letters, **9** (2009) 4221.
[3]. E. Della Gaspera *et al*. Advanced Functional Materials, **25** (2015) 7263.
[4]. T. W. Kim and K.-S. Choi, Science, **343** (2014) 990.
[5]. T. Yajima *et al*. Nature Chemistry, **7** (2015) 1017.

Contact Details:
To discuss this project further please contact:
Dr. Enrico Della Gaspera (enrico.dellagaspera@rmit.edu.au) 1st Supervisor – Office 3.2.7

Enzyme Biocatalysis in Ionic Liquids

Applied Chemistry and Environmental Science Discipline - RMIT City

Project Description

This project will involve developing new non-aqueous solvents for biocatalysis reactions. Biocatalysts are highly useful in the synthesis of many organic compounds and chemical transformations. However, they are typically limited to use in conditions similar to their natural environment (ie. aqueous conditions, room temperature and at neutral pH). There are potentially new uses for them if we can develop solvents which support enzyme activity across a broader range of solvent conditions.[1]

The solvents to be used in this project will predominantly be protic ionic liquids (PILs), which are liquid salts below 100 ^{o}C. PILs are "designer" solvents due to their high tailorability. They consist of a cation and an anion, and there are thousands of possible combinations, with structural changes leading to changes in their chemical, thermal and solvent properties.[2] Previously ionic liquids have been shown to have either a stabilising or destabilising effect on proteins, depending on their ions, concentration and which proteins.[3-4]

Libraries of PILs will be designed based on the groups previous experience in this field, and these will be synthesised using a Chemspeed robotic platform.[5] Commercially available enzymes will be used which are commonly used in organic synthesis. A large range of physical chemistry techniques will be used to characterise the chemical, solvent and thermal properties of the neat PILs. Similarly, a variety of techniques will be used to characterise the enzymes in the PILs, and to monitor the biocatalysis reactions in the PILs. These techniques will include NMR, FTIR, differential scanning calorimetry (DSC), Small and Wide angle X-ray scattering at the Australian Synchrotron (SAXS/WAXS), UV-Vis spectroscopy, as well as measurements of surface tension, density and viscosity.

The aim of this project is to identify which PILs, and PIL solvent features, are beneficial for supporting different types of enzymes for biocatalysis reactions.

The research environment for this project is dynamic, friendly and supportive. It would give the successful candidate great opportunities for development, such as in research, communication, organisation, project management, problem-solving and analysis skills. The supervisors have a high international reputation in this field, and strong publication records.

References:
1.Schmid, A.; Dordick, J. S.; Hauer, B.; Kiener, A.; Wubbolts, M.; Witholt, B., *Nature* **2001,** *409*, 258-268.
2.Greaves, T. L.; Drummond, C. J., *Chem. Rev.* **2015,** *115*, 11379-11448.
3.Wijaya, E. C.; Separovic, F.; Drummond, C. J.; Greaves, T. L., *Phys. Chem. Chem. Phys.* **2016,** *18*, 25926-25936.
4.Zhao, H., *Journal of Chemical Technology and Biotechnology* **2010,** *85* (7), 891-907.
5.Greaves, T. L.; Ha, K.; Muir, B. W.; Howard, S. C.; Weerawardena, A.; Kirby, N.; Drummond, C. J., *Phys. Chem. Chem. Phys.* **2015,** *17*, 2357-2365.

Contact Details:
To discuss this project further please contact:

Dr Tam Greaves (tamar.greaves@rmit.edu.au) 1st Supervisor – Office 3.2.05B
Prof Calum Drummond (calum.drummond@rmit.edu.au) 2nd Supervisor

DR229 – PhD (Applied Chemistry)
MR229 – Master of Science (Applied Chemistry)

School of Science HDR Project 2018

Interaction of novel cryoprotectants and model membranes

Applied Chemistry and Environmental Science Discipline/(Marine and Terrestial Natural Product (MATNAP) Research Group) – RMIT City

Project Description

Cryopreservation of cells involves storing the cells at very cold temperatures to minimise activity and prevent damage to the cells. However, the freezing process is very risky for cells, and requires cryoprotectants and tailored freezing protocols to enable cells to survive and not dehydrate or burst. Cryoprotectants are additives which allow cells to avoid intra-cellular ice formation, encourage the formation of a glass at low temperatures, and minimize dehydration damage. Thus effective cryoprotectants must have the following properties [1]:

i) They must be able to permeate the cell membrane to become internalised
ii) They must discourage ice formation
iii) They must have minimal toxicity to cells
iv) They must be able to vitrify (ie form a glass) at low temperatures

However, there are currently few successful cryoprotectants, and few cells which can be successfully frozen, so there is a strong need for a wider variety of cryoprotectants.

This project will involve developing novel molecules and compounds which are potentially good cryoprotectants. Novel cryoprotectants of ionic liquids [2] and sugars, along with existing cryoprotectants, such as DMSO, glycerol and ethylene glycol will be used. The glass forming properties of each of these additives neat, and in water, will firstly be characterised using differential scanning calorimetry (DSC).

The interactions of these cryoprotectants will be investigated with artificial model cell membranes made from lipid bilayers. The location of cryoprotectants in the membrane, interactions between the cryoprotectants and membrane, and effect on the membrane structure will be explored. The techniques to be used include small angle X-ray scattering (SAXS), small angle neutron scattering (SANS) [3], and infrared spectroscopy. Some of these experiments will be conducted using national or international Synchrotron or Neutron scattering research facilities.

The key aim of this project is to develop fundamental understanding of how cryoprotectants interact with membranes, including their permeability, toxicity, and location within the membrane, and to leads to new, novel cryoprotectants.

References

[1] Wolfe, J., Bryant, G. Cryobiology **1999**, *39*, 103-129.
[2] Greaves, T. L.; Drummond, C. J., *Chem. Rev.* **2015,** *115*, 11379-11448.
[2] Kent, B., Hauß, T., Demé, B., Cristiglio, V., Darwish, T., Hunt, T., Bryant, G., Garvey, C.J. Langmuir **2015**, *31*, 9134-9141.

Contact Details

To discuss this project further please contact:

Dr Tam Greaves (tamar.greaves@rmit.edu.au) Supervisor – Office 3.2.05B
Prof Gary Bryant (gary.bryant@rmit.edu.au) Supervisor – Office 14.7.6

Conotoxins as Potential Novel Therapeutics for Neuropathic Pain

Applied Chemistry and Environmental Science Discipline - RMIT / University of Wollongong

Project Description

Neuropathic pain is characterized by the chronic sensation of physical pain in the absence of noxious external stimuli, and is a multifaceted disease involving dysfunction of a number of neuronal proteins, including nicotinic acetylcholine receptors (nAChRs), voltage-gated sodium (Na^+) and calcium (Ca^{2+}) ion channels. One rich source of peptide-based therapeutics for treatment of neuropathic pain is the conotoxins: small, cysteine-rich bioactive peptides derived from the venom of tropical marine *Conus* snails. Conotoxins have a wide range of pharmacological targets, including different isoforms of ion channels and membrane receptors. Thus, conotoxins are useful research tools and promising drug leads for diseases related to these targets, especially disorders of the nervous system. This is evidenced by the production of Ziconotide (ω-conotoxin MVIIA), which has been approved by the US FDA as a local analgesic for severe chronic pain treatment.

A number of different conotoxin scaffolds have been identified, each defined by their structure, target, and mode of inhibition. The *ψ-conotoxin* PIIIE acts as a non-competitive antagonist of the muscle-type nAChR. The largest family are the *α-conotoxins*, which have been shown to be competitive antagonists of nAChRs, and can be further divided into structural subfamilies depending on the number of amino acids between two clusters of cysteine residues. A growing library of natural and synthetic α-conotoxins have been identified which exhibit selective potency against subtypes of nAChRs. Finally, *μ-Conotoxins* comprise 16 to 26 residues, and are the only venom peptides that selectively inhibit voltage-gated Na^+ channels by blocking ion flux via binding to the outer vestibule of the channel. The μ-conotoxin GIIIA was among the first to be characterized, and preferentially blocks skeletal muscle sodium channel NaV1.4 by complex toxin–pore interactions. Recent experiments also demonstrated μ-conotoxin inhibition of voltage-gated Ca^{2+} channels which, along with nAChRs and Na^+ channels, are also important for pain sensation in disease models.

The main aim of this collaborative project is to use computational molecular modeling and simulation methods to identify the binding modes and specific inter-residue interactions between a range of conotoxin families and their known receptor targets, with especial focus on interactions between α-conotoxins with nAChRs and the μ-conotoxins with Na^+ and Ca^{2+} ion channels. Simulations will also be used to examine the detailed mechanisms of their functional effects on their targets, while binding free energy calculations will be used to aid in the design of novel conotoxin analogues with enhanced selective potency against specific subtypes of target neuronal proteins. This project will ultimately aid in the production of novel conotoxin-based therapeutics with enhanced selectivity, potency, and efficacy in the treatment of chronic pain.

References:

[1]. "Molecular simulation study of the unbinding of [γ4E]-GID at the α7 and α4β2 nicotinic acetylcholine receptors", **Hung, A.**, Suresh, A. (2016) *Journal of Molecular Graphics and Modelling*, 70, 109-121

[2]. "Molecular Basis for Differential Sensitivity of α-Conotoxin RegIIA", Kompella S.N., Cuny H., **Hung A.**, **Adams D.J.** (2015) *Molecular Pharmacology*, 88(6), pp. 993-1001.

[3]. "Dicarba α-Conotoxin Vc1.1 Analogues with Differential Selectivity for Nicotinic Acetylcholine and GABAB Receptors", van Lierop, B.J., Robinson, S.D., Kompella, S.N., Belgi, A., McArthur, J.R., **Hung, A.**, MacRaild, C.A., **Adams, D.J.**, Norton, R.S., Robinson, A.J. (2013), *ACS Chemical Biology*, 8 (8), 1815–1821

Contact Details:

Dr Andrew Hung (andrew.hung@rmit.edu.au) 1st Supervisor - RMIT
Prof David Adams (djadams@uow.edu.au) 2nd Supervisor - University of Wollongong

Molecular mechanisms of action of dietary antioxidants and chromatin modifying compounds

Applied Chemistry and Environmental Science Discipline – RMIT City/Monash University

Project Description

The medicinal properties of the leaves and fruit of *Olea europaea* (olive tree) have been known since antiquity, and consumption of olive oil has been associated with a decreased risk of cardiovascular disease and certain cancers. Increasingly, there is interest in the biological properties of the molecular constituents of olives. For example, hydroxytyrosol has been shown to be a potent antioxidant and has anti-atherogenic and anti-cancer properties. However, the specific constituents responsible for various beneficial effects of olives, as well as their molecular targets, are not well known. The main aim of this project is to use molecular computational modeling and simulation methods to identify key molecular targets of specific bioactive components of olives, and to produce molecular-level characterisation of their mechanisms of action. The outcomes of this project will aid development of novel therapies derived from dietary compounds, which may have substantial advantages over synthetic drugs, including lower dosage requirements and reduced risk of adverse side effects. This project will focus on identifying the mechanisms of action of dietary olive compounds on two specific areas:
1) *Epigenetic control*: Controlled equilibrium between histone acetylation and deacetylation is essential for normal cell growth, and perturbations have been associated with various diseases. Although numerous compounds have been developed to specifically alter the function of chromatin modifying enzymes (eg. histone deacetylase inhibitors have emerged as potential cancer chemo-therapeutics), we are only at the early stages of understanding the epigenetic effects of dietary compounds. This project area will involve use of computational biophysics approaches, combined with known experimental affinities, to identify potential chromatin modifying compounds derived from *Olea europaea*. This project will also involve experimental validation of targets using *in vitro* binding and enzyme activity inhibition assays and identify potential epigenetic effects in a clinical context. 2) *Inflammation*: Non-steroidal anti- inflammatory drugs (NSAIDs) are among the most widely used therapeutic agents around the world, commonly used to reduce pain. However, there are adverse effects with the use of NSAIDs, including gastrointestinal bleeding and cardiovascular effects. Hence, there has been a rise in the development of alternatives to traditional NSAIDs. A previous study found that oleocanthal, a phenolic compound derived from olive, had similar effects to ibuprofen, a commonly used NSAID. But there is a multitude of additional compounds in olive that have yet to be investigated. Hence, this project will study the mechanisms of olive derived compounds in inflammation using molecular computational modeling and simulation approaches. Enzymes involved in inflammation pathways will be explored as potential targets for olive-derived compounds. Elucidation of the mechanism of action on these proteins will be valuable in developing novel drugs for the treatment of inflammation.

References:

[1]. "Exploration of mechanisms in nutriepigenomics", Bonvino, N. P., Liang, J., **Hung, A. & Karagiannis, T.** (2015) *Hellenic Journal of Nuclear Medicine*. 18, Suppl 1, p. 51-62

[2]. "The Implication of Cancer Progenitor Cells and the Role of Epigenetics", Tortorella, S. M., **Hung, A. & Karagiannis, T. C.** (2015) *Antioxidants and Redox Signaling*. 22, 16, p. 1425-1462

[3]. "Cellular and Molecular Effects of Bioactive Phenolic Compounds in Olives", Ray, N. B., Bonvino, N. P. & **Karagiannis, T. C.** (2015) *Olive and Olive Oil Bioactive Constituents.* Boskou, D. (ed.). Netherlands: Elsevier, p. 53-91

Contact Details:

Dr Andrew Hung (andrew.hung@rmit.edu.au) 1st Supervisor - RMIT
Dr Tom Karagiannis (tom.karagiannis@monash.edu) 2nd Supervisor - Monash University

Applied Electrochemistry: New Nanostructured Materials for Energy Conversion.

Applied Chemistry and Environmental Science Discipline/CAMIC (Centre for Advanced Materials and Industrial Chemistry) – RMIT City

Project Description

Electrocatalysis in energy conversion, or electroanalysis using metal based nanoparticles or porous alloys is an area intensive research, as there are still fundamental gaps in our knowledge for the complete understanding of what happens on the surface of a nanostructured material during an electrochemical process.

In this project **new nanostructured materials will be designed and prepared**, based on porous noble metal based materials (Au, Pt,….), or supported nanoparticles of precisely defined shape and chemistry, and tested for **emerging electrocatalytic reactions** in modern materials science: such as the complex conversion of molecules such as SO_2 or CO_2.

The project will involve the design and fabrication of nanostructured catalysts based on noble metals by electrodeposition, with control of both nanostructure and surface chemistry. Advanced electrochemical cells will be built from concept to implementation in-house, to directly study the surface chemistry of these materials *in situ* during catalysis, using advanced techniques such as *in situ* Raman spectroscopy, on line mass spectrometry. This will offer new insights into the complex catalytic electrochemical processes taking place, allowing better electrocatalysts to be developed .

This project will thus develop new, exciting techniques to study the surface behaviour of nanostructured inorganic materials, provide new insights in to the catalytic mechanisms with applications in energy (fuel cells, battery technology), sensing (electrocatalytic analysis of analytes) and fundamental theories (corrosion theory), giving the student exposure to all of the broad techniques used modern electrochemical science.

Dr. Jones has strong links with CSIRO, Industry, and other Australian Universities through the CAMIC research centre, giving the student opportunities to collaborate with other scientists in a multidisciplinary team, and receive a comprehensive training in modern materials science.

References from our Group:
[1]. Building with bubbles: the formation of high surface area honeycomb-like films via hydrogen bubble templated electrodeposition, BJ Plowman, Lathe Jones* SK Bhargava*, *Chemical* Communications 51 (21), 4331-4346, **2015**
[2]. The Preparation of a AuCN/Prussian Blue Nanocube Composite through Galvanic Replacement Enhances Stability for Electrocatalysis, B Ren, Lathe Jones*, DK Oppedisano, AE Kandjani, M Chen, F Antolasic, ...*ChemistrySelect* 2 (19), 5333-5340, **2017**.

Contact Details:
To discuss this project further please contact:
1st Supervisor – Dr. Lathe Jones, lathe.jones@rmit.edu.au. Room 3.02.04.
2nd Supervisor – Dr. Ahmad Kandjani, ahmad.kandjani@rmit.edu.au

The Electrochemical Study of the Mineral Surfaces with Micron Resolution.

Applied Chemistry amd Environmental Science/CAMIC (Centre for Advanced Materials and Industrial Chemistry) – RMIT City

Project Description

The minerals industry is an important economic contributor to Australia, however high-grade reserves have been progressively depleted, leaving predominantly low grade ores (i.e. ores with a low valuable metal content). Exploitable copper ore grades are now invariably in the range 1% Cu and below, and Uranium reserves are often complicated by refractory ores that are difficult to extract. Approximately 80 % of copper is extracted using conventional smelter technology, which has a significant environmental footprint (e.g. slag production, dust and SO_x emissions), and is not cost effective for low grade copper sulphide ores.

Heap leaching of such ores could be the most **sustainable, economical method to recover copper**, but is prevented by **knowledge gaps in our fundamental understanding** of copper sulphide and refractory Uranium mineral dissolution.

In this project, long standing questions relating to the **fundamental reasons** for the **slow leaching of minerals such as Chalcopyrite** and **Uranium ores** will be addressed, thus developing technology to access technically difficult ore bodies.

A new class of microelectrodes will be fabricated by Advanced Manufacturing Methods, and the technique of Scanning Electrochemical Microscopy (SECM) will be used study the surface of ores with micron resolution, allowing leaching of individual grains of ore, and also the study of activity at grain boundaries to a level of detail that has not been possible before. This will be supplemented by the surface characterisation via modern techniques such as SEM, In-situ Raman, and synchrotron science, in collaboration with our contacts at CSIRO and several large multinational mining companies. The student will graduate with a broad perspective of the fundamental and applied challenges facing modern inorganic and minerals scientists.

Our References:

[1]. Probing the Surface Chemistry of Uranium Refractory Ores with a Microelectrode, L Jones, R Ram, J Tardio, M Pownceby, M Chen, S Bhargava, *SAIMM Hydrometallurgy*, 163, **2016**

[2]. A review of acid leaching of uraninite, SK Bhargava, R Ram, M Pownceby, S Grocott, B Ring, J Tardio, L Jones, *Hydrometallurgy* 151, 10-24, **2015**

Contact Details:

To discuss this project further please contact:

1st Supervisor – Dr. Lathe Jones, lathe.jones@rmit.edu.au

2nd Supervisor – Prof. Suresh Bhargava, suresh.bhargava@rmit.edu.au

DR229 – PhD (Applied Chemistry)
MR229 – Master of Science (Applied Chemistry)

School of Science HDR Project 2018

Design of Nanosized ceria-based Materials for Catalytic Oxidation Reactions

Applied Chemistry and Environmental Science Discipline/CAMIC/Chemical Sensor Group – RMIT City

Project Description

Nanostructured Ceria (CeO2) based materials have attracted significant interest in the present frontier research for their wide applications in heterogeneous catalysis. Particularly, the use of ceria in the domain of environmental catalysis is due to its superior chemical and physical stability, and a large number of oxygen vacancies (involving facile Ce^{4+}/Ce^{3+} redox chemistry) and their mobility, which are the main characteristic features of the fluorite-type oxides. Although, its inherent chemical properties such as high oxygen storage capacity and high oxygen mobility originating from facile Ce^{3+}/Ce^{4+} redox cycle dominate its use, its functional performance is further influenced by its size, morphology and structure, and surface area..

The main focus of this project is to develop various ceria-based materials for different catalytic applications such as Hg^0 oxidation, soot oxidation, and degradation of organic pollutants. Among these three applications, primarily, the Hg^0 oxidation studies will be done thoroughly over different ceria-based materials under different flue gas conditions such as HCl, O_2, HCl/O_2-mix, and NH_3. Also an attempt will been carried out to expand the work to utilize the ceria-based materials for other well-known applications like catalytic soot oxidation and photocatalysis.

This is a collaborative project with CSIRO and RMIT and will give the student opportunity to work with scientists from diverse backgrounds.

References:

1. Y. Shijian, G. Yongfu, Y. Naiqiang, W. Daqing, H. Hongping, Q. Zan, and J. Jinping Ind. Eng. Chem. Res. 2011 50 (16) 9650-9656.
2. D. Jampaiah, K. M. Tur, S. J. Ippolito, Y. M. Sabri, J. Tardio, S. K. Bhargava and B. M. Reddy, RSC Adv., 2013, 3, 12963–12974.
3. A. A. Presto, E. J. Granite, A. Karash, R. A. Hargis, W. J. O'Dow and H. W. Pennline, Energy Fuels, 2006, 20, 1941– 1945.
4. A. P. Jones, J. W. Hoffmann, D. N. Smith, T. J. Feeley and J. T. Murphy, Environ. Sci. Technol., 2007, 41, 1365–1371.

Contact Details:

To discuss this project further contact:

Dr Ylias Sabri (ylias.sabri@rmit.edu.au) 1st Supervisor–Office 3.01.04
Dist. Prof. Suresh Bhargava (suresh.bhargava@rmit.edu.au) 2ndSupervisor–Office 3.01.04

UV-assisted solid-state gas sensors for non-invasive diagnostic applications

Applied Chemistry and Environmental Science Discipline/CAMIC/Chemical Sensor Group – RMIT City

Project Description

Widespread screening for lung cancer by novel non-invasive methods can drastically increase early-stage diagnosis. This can improve long-term survival rates from less than 6% to 35% with the potential to reduce the yearly worldwide lung cancer mortality rate of 1.3 million by one third [1]. Among non-invasive screening methods, breath composition analysis is a low-cost alternative to blood analysis that can detect early-stage lung cancer [1]. However, its application to healthcare is currently restrained by the lack of portable technologies having sufficient selectivity and sensitivity for the real-time measurement of the marker molecules in complex gas mixtures such as the breath.
Here, we will develop a novel gas molecule sensing technique to enable real-time measurement of breath markers. We will do this by exploiting the ability of plasmonic nanostructures to selectively absorb light and transfer its energy to drive chemical reactions on the surface of a nearby semiconductor nanoparticle. Integrating such plasmonic light absorbers into highly sensitive (semiconductor) gas sensors [2] will provide a means to selectively promote oxidation or reduction of the target molecules. This will be achieved by tuning the light absorption wavelength to match the activation energy of the desired (gas sensing) reactions. Enabling selective measurement of volatile organic compounds (VOCs) in human breath by low-cost semiconductor technology could revolutionize modern healthcare through early-stage diagnosis and self-monitoring of a wide range of medical conditions.

This is a recently awarded ARC-Discovery project in collaboration with ANU and QUT thus giving students opportunity to travel to different universities and meet scientists and students from different disciplines while undertaking experimental work.

References:

[1] G. Peng, U. Tisch, O. Adams, M. Hakim, N. Shehada, Y. Y. Broza, S. Billan, R. Abdah-Bortnyak, A. Kuten, H. Haick, Nature Nanotech. 2009, 4, 669.
[2] A. Tricoli, S. E. Pratsinis, Nature Nanotech. 2010, 5, 54.
[3] A. Tricoli, M. Graf, S. E. Pratsinis, Adv. Funct. Mat. 2008, 18, 1969.
[4] M. Righettoni, A. Tricoli, S. E. Pratsinis, Chem. Mat. 2010, 22, 3152.

Contact Details:

To discuss this project further contact:

Dr Ylias Sabri (ylias.sabri@rmit.edu.au) 1st Supervisor– 3.01.04
Dr Samuel Ippolito (samuel.ippolito@rmit.edu.au) 2nd Supervisor– 10.07.06
Dr Ahmad Kandjani (ahmad.kandjani@rmit.edu.au) 2nd Supervisor– 3.01.04

School of Science HDR Project 2018

Colloidal lithography based nanostructures for numerous applications.

Applied Chemistry and Environmental Science Discipline/CAMIC/Chemical Sensor Group

Project Description

To date there is a technological demand for the fabrication of structures where both the feature size and separation can be controlled at the nanoscale. Typically such structures are obtained by direct writing using electron beam lithography, but the method is sequential and thus slow and not cost-effective. An alternative strategy exploits the deposition of colloidal particles as masks for lithography. Colloidal lithography is a large-area, robust, parallel and cheap method, but conventional approaches have little control on the inter-particle separation, typically yielding close-packed particle arrays. For instance, in biosensing applications, large separations compared to the feature size are necessary to avoid cross-talk between neighboring sensing spots. As another example, nanofabricated arrays of silicon nanowires have significant potential as platforms for cell transfection or as materials for optics and energy applications, but their diameter, height and lateral separation need to be finely tuned to achieve the desired final properties.

In our group we harness and exploit the self-assembly of colloidal particles at a water/oil interface to meet these challenges. After self-assembly at the liquid interface, the colloidal particle arrays can be deposited on a solid substrate for lithography. The technique allows in a single step to produce 2D patterns where the size of the features and their separation can be controlled independently and has been used to produce nanopore arrays, biosensing structures, nanopatterned hydrogels, porous polymer membranes and nanowire arrays out of different materials.

This is an emerging field and the student will be able to produce a range of novel structures for applications ranging from gas sensing to solar energy harvestation, electrochemistry, catalysis and the like.

References:

[1] YM Sabri, AE Kandjani, SJ Ippolito, SK Bhargava, Scientific reports 6, 24625
[2] YM Sabri, AE Kandjani, SJ Ippolito, SK Bhargava ACS applied materials & interfaces 7 (3), 1491-1499.

Contact Details:

To discuss this project further contact:

Dr Ylias Sabri (ylias.sabri@rmit.edu.au) 1st Supervisor– 3.01.04
Dr Lathe Jones (lathe.jones@rmit.edu.au) 2nd Supervisor– 3.03.06A
Dr Ahmad Kandjani (ahmad.kandjani@rmit.edu.au) 2nd Supervisor– 3.01.04

Building with smoke

Applied Chemistry and Environmental Science Discipline/CAMIC/Chemical Sensor Group – RMIT City

Project Description

Carbon soot is one of the oldest materials known for its hydrophobic properties, robustness, and availability, making it an ideal material for use in various applications. The drawbacks, however, are the loose structural binding between constructing carbon nanoparticles and the amorphous nature of soot itself. In this project, the student will investigate a facile chemical vapor deposition (CVD) method that maintains the soot template structural integrity and enables its modification into a highly photoactive, self-cleaning titania fractal network. We have previously shown that such technique results in surfaces with small air pockets that are available on the surface combined with the salinization process producing TiO_2 fractal network with superamphiphobic properties. Given the high surface area of the fractal network structure and titania's well-known photocatalytic activity, the designed surfaces can be assessed for their photocatalytic decoloration activities. Soot template derived TiO_2 films can offer enormous potential in many different applications where self-cleaning and/or high surface area and photoactive properties are required. When modified with other metal/metal oxide decoration techniques, these surfaces could be highly active for catalysis and chemical/biochemical sensing applications. The student will have an opportunity to explore a large combination of materials with different properties for a wide range of applications.

This is an emerging field and the student will be able to produce a range of novel structures for applications ranging from gas sensing to solar energy harvestation, electrochemistry, catalysis and the like.

References:
[1] AE Kandjani, YM Sabri, MR Field, VE Coyle, R Smith, SK Bhargava, Chemistry of Materials 28 (21), 7919-7927

Contact Details:
To discuss this project further contact:
Dr Ahamd Kandjani (ahmad.kandjani@rmit.edu.au) 1st Supervisor– 3.01.04
Prof Suresh Bhargava (suresh.bhargava@rmit.edu.au) 2nd Supervisor– 3.01.04A
Dr Ylias Sabri (ylias.sabri@rmit.edu.au) 2nd Supervisor– 3.01.04

School of Science

Molecular biology meets Nanotechnology: An accurate, point-of-care diagnosis and bio-control for the pathogens causing Powdery Mildew and Botrytis in Grapes

Discipline: Biosciences and Food Technology/Applied Chemistry and Environmental Science.
Centre for Environmental Sustainability and Remediation
Location (City and Bundoora)

Project Description

Powdery mildew [1] represents in economic terms the most important disease affecting the grape industry world-wide which costs Australia AUD $140 million per annum. Botrytis is the second most important disease, behind powdery mildew. The economic impact through increased vineyard costs, yield loss and reduced income was estimated at $52 million per annum. Currently chemical fungicides are routinely used for the control of these plant pathogens. However, fungal resistance and residual fungicide present on the grape are major global current concerns. To date no alternative eco-friendly strategy exists that offers complete control of these plant pathogens.
The Food and Agriculture Organization of the United Nations (FAO) indicates that about 33 percentage of global agriculture (including viticulture) production is lost or wasted annually. Therefore by reducing waste (providing biosecurity), this project could lead to an increase efficiency for the Australian wine industry and avoid the loss of resources. The worldwide market for the treatment of mildews and botrytis in grapes currently stands around $ AUS 1.2 billion. This PhD project will have a significant impact on the Australian Wine Industry. In this project the objectives are to:

- Develop protocols for synthesis of various nano-formulations, their characterization and assessment of anti-microbial activity and mechanisms against model agricultural pathogens.
- Develop large scale synthesis protocols for nano-formulations and optimization of their long term storage capacity.
- Optimization and demonstration of a novel, convenient and rapid single tube multiplex Recombinase Polymerase Amplification (RPA)-Lateral Flow Strip assay [2] for the detection of Powdery mildew [*Erysiphe necator* (syn. *Uncinula necator*)] and Botrytis (*Botrytis cinerea*) outside of a laboratory setting that can detect the pathogen accurately.

Given the interdisciplinary nature of the project (and funded by Bridging grant, Global Connection Fund, ATSE and the AusIndustry) students will receive training across a number of subject fields, including agricultural nanotechnology, nano-toxicology, materials science, advanced molecular biology and bio-sensing. Students will also have access to state-of-the-art biological characterisation laboratory at the Microbial Life Laboratory, Bundoora and the RMIT MicroNano Research Facility, and the advanced material characterization tools (atomic force microscopy, transmission electron microscopy, dynamic light scattering, X-Ray photoemission spectroscopy, inductively coupled plasma mass Spectroscopy, X-Ray diffraction) at the RMIT Microscopy & Microanalysis Facility and Applied Chemistry advanced instrumentation facility. There are no ethical concerns need to be addressed for this project.

References:

[1]. Wenping Qiu *et al.*Horticulture Research, 2, (2015), 15020
[2]. Kui Sun *et al.* Parasites & Vectors, 9 (2016) 476

Contact Details:

To discuss this project further please contact:

Dr Sarvesh K Soni (sarvesh.soni@rmit.edu.au) 1st Supervisor – 3 992 56678
Dr Selvakannan Periasamy (selvakannan.periasamy@rmit.edu.au) 2nd Supervisor – 3 9925 0805

Self-assembled lipid nanoparticles for targeted cancer therapeutics

Applied Chemistry and Environmental Science Discipline - RMIT City

Project Description:

Cancer is a leading cause of the death and a major health problem in Australia. Currently, chemotherapeutics are widely used and still provide the best survival chance for cancer patients. Chemotherapy drugs, however, also damage normal cells in the body, leading to many side effects that have been limiting their effectiveness. To address these problems, nanomedicines, a drug delivery strategy based on nanoparticles encapsulating toxic chemotherapeutics, have emerged and held great promises for the next generation of targeted cancer treatment to reduce systemic side effects. Such drug delivery systems also offer other advantages including: (1) enhanced solubility of newly discovered, poorly soluble drugs, (2) controlled release of the drugs for enhanced bioavailability (3) protection of the drugs from degradation in the body to overcome biological barriers.

Among the drug delivery systems that are being developed, self-assembled lipid nanoparticles stand out due to their customizable nanostructures and extensive porous networks. These features allow them to encapsulate and slowly release non-water-soluble chemotherapeutics.[1] We have also successfully attached antibodies to the surfaces of lipid nanoparticles to help them recognise cancer cells for targeted drug delivery.[2]

This project aims to formulate multifunctional lipid nanoparticles that can provide sustained release and targeted delivery of anti-cancer chemotherapeutic drugs, including paclitaxel, temozolomide, and dasatinib. Extensive investigation of structure – function relationship between lipid nanostructures and solubility and release of drugs will be performed *in vitro* and *in vivo*. First, advanced biophysical techniques such as small angle X-ray scattering, cryogenic transmission electron miscroscopy, HPLC will be employed. Second, biochemical assays such as bioconjugation, gel electrophoresis, ligand binding assays, *in vitro* cell viability and cell uptake assays will also be performed to confirm the recognition of cancer cells by nanoparticles. Last but not least, biological functions and therapeutic efficacy of the developed nanoparticles will be evaluated *in vivo* using ovarian cancer and/or brain cancer xenograft models.

This project is a collaborative interdisciplinary project that offers training on lipid nanoparticle formulation, colloid and surface chemistry characterisation, and the evaluation of bio-nanomaterials *in vitro* and *in vivo*.

References:

[1]. X. Mulet, B. J. Boyd, C. J. Drummond, Journal of colloid and interface science 2013, 393.
[2]. J. Zhai: Nanoscale, 2015, 7, pp. 2905-2913

Contact Details:

To discuss this project further please contact:

Dr Nhiem Tran (nhiem.tran@rmit.edu.au) 1st Supervisor (Joint) – Office 3.2.22
Dr Jiali (Maggie) Zhai (maggie.zhai@rmit.edu.au) 1st Supervisor (Joint) – Office
Professor Calum Drummond (calum.drummond@rmit.edu.au) 2nd Supervisor

Antimicrobial coating for orthopaedic implants

Applied Chemistry and Environmental Science Discipline/School of Engineering – RMIT City

Project Description:

Orthopaedic implants are regularly used to fix a large number of fractures occurred worldwide. However, implant loosening due to lack of bone ingrowth and infection are among the most common causes of orthopaedic implant failure.[1] The situation worsens by the quick emergence of antibiotic resistant bacteria. This project focuses on the development of polymer – transition metal oxide hybrid coatings for orthopaedic implants. The hybrid coatings combine the flexibility of polymer and bioactivity of metal oxide. Furthermore, the addition of antibacterial agents in the coating can lead to sustained release of these compounds.[2] The desirable coatings should improve bone cell function, reduce inflammatory reaction, and prevent the formation of bacterial biofilm. Antimicrobial metal and metal oxide (such as silver and zinc oxide) and antimicrobial peptides are of main focus as they have shown to be more difficult for bacteria to develop resistance. The coating will be optimised by varying the formulation compositions to achieve a strong mechanical bond to the implant, enhanced bone cell functions, and sustained release of antimicrobial agents at inhibitory doses.

RMIT has been at the forefront of 3D printing techniques that allow for the fabrication of personalised orthopaedic implants.[3] It is therefore critical to also evaluate coating techniques (i.e. dip coating, spin coating, and plasma spraying) that are suitable for these novel 3D printed implants.

The HDR candidate will gain experience in an interdisciplinary field that include surface and interface chemistry, materials science, nanoengineering, and biomedical engineering. The coatings will be fabricated using a modified sol-gel process. The coatings will be studied by various surface characterisation techniques, such as scanning electron microscopy, atomic force microscopy, and X-ray photoelectron spectroscopy. Subsequently, their bioactivity and toxicity will be studied by examining bone-forming cell viability and function on the coated surfaces. Moreover, the ability of the coating to resist bacterial colonisation will be assessed against common pathogens including *Staphylococcus aureus*, *E. coli*, and *Pseudomonas aeruginosa*.

References:

[1]. Campoccia D, et al., Biomaterials, 2006, 27(11): 2331-2339
[2]. Tran N, Kelley M, et al. Mat Sci Eng: C, 2015, 49: 201-209
[3]. Wang X et al., Biomaterials, 2016, 83:127-141

Contact Details:

To discuss this project further please contact:

Dr Nhiem Tran (nhiem.tran@rmit.edu.au) 1st Supervisor – Office 3.2.22
Dr Kate Fox (kate.fox@rmit.edu.au) 2nd Supervisor – Office 57.3.16

DR229 – PhD (Applied Chemistry)
MR229 – Master of Science (Applied Chemistry)

School of Science

HDR Project 2018

Lyotropic liquid crystalline nanomaterials for encapsulation and delivery of siRNA

Applied Chemistry and Environmental Science Discipline - RMIT City

Project Description:

RNA interference (RNAi) therapeutics is a fast growing field with the potential to revolutionize current treatments for significant diseases including cancer, autoimmune dysfunction, and various genetic disorders. This technology relies on the repression of disease proteins using small interfering RNAs (siRNA), which can be designed for a specific disease. In the cell cytoplasm, siRNA are incorporated into the RNA-induced silencing complex (RISC), which identifies and degrades the complementary messenger RNA that is responsible for protein production.[1] However, siRNA are large polyanionic molecules which are easily degraded by nuclease. In order to effect changes to the cell, they must be transported across the cell membrane and released into the cell cytoplasm. Lyotropic lipid nanoparticles consisting of cationic lipids are highly prospective delivery vehicles for siRNA. In excess water, lipid molecules self-assemble into nanoparticles with unique internal nanostructures. [2] These materials have been studied as drug delivery vehicles due to their ability to incorporate both hydrophilic and lipophilic molecules.[3]

This project aims to study the influence of physicochemical factors such as surface charge, critical packing parameter of lipid molecules, and membrane curvature on the internal structure of the nanoparticles, and their ability to encapsulate and release siRNA. Extensive nanoparticle characterisation will be performed using small angle X-ray scattering (SAXS), cryogenic transmission electron microscopy (cryo-TEM), and dynamic light scattering techniques (DLS). In vitro cytotoxicity and gene knockdown experiments will be carried out.

Skills: Understanding of colloid and surface chemistry. Structural characterisation of bio-nanomaterials. Willingness to work on a collaborative interdisciplinary project.

References:

[1]. G. Meister, T. Tuschl, Nature 2004, 431, 343.
[2]. C. Fong, T. Le, C. J. Drummond, Chemical Society Reviews 2012, 41, 1297.
[3]. X. Mulet, B. J. Boyd, C. J. Drummond, Journal of colloid and interface science 2013, 393.

Contact Details:

To discuss this project further please contact:

Dr Nhiem Tran (nhiem.tran@rmit.edu.au) 1st Supervisor – Office 3.2.22 *Dr Charlotte Conn* (charlotte.conn@rmit.edu.au) 1st Supervisor – Office

Bioactivity assessment of natural products derived from Australian Terrestrial and Marine organisms and Exploration of Chemical Separation Methodologies

Applied Chemistry and Environmental Science Discipline/(Marine and Terrestial Natural Product (MATNAP) Research Group) – RMIT City

Project Description

The proposed research will involve the extraction of a range of marine and terrestrial organisms with a focus on isolating biologically active compounds.[1-2] The study will focus on the chemical diversity of marine organisms and the ethnopharmacology of Australian terrestrial organisms.

Selected organisms will be targeted for extraction. Crude extracts of these organisms will be further fractionated using organic solvents and then further analysed via analytical HPLC in order to assess viability for further isolation. Often the fractions will be investigated further using hyphenated spectroscopic techniques such as HPLC-NMR and HPLC-MS to quickly ascertain the nature of the secondary metabolites or natural products present.[3] This is a rapid chemical screening method. Initially crude extracts of all marine and terrestrial samples will be subjected to a variety of chromatographic techniques followed by High Pressure Liquid Chromatography (HPLC) for further purification. This project will also involve adapting the use of 2D HPLC as a means to further resolve closely eluting natural products.

All isolated compounds are identified via a series of analytical techniques. Initially UV/Visible spectra obtained via Photo Diode Array (PDA) detection from analytical HPLC will be utilised. This provides valuable information on whether the compound possesses a characteristic UV chromophore and can be an aid to quickly deducing a compound’s structure class. A large array of NMR experiments and mass spectrometry are employed in the structure characterisation process. Through an existing collaboration with The University of Melbourne compounds that provide stable crystal structures can be analysed via X-Ray Diffraction (XRD) to obtain a complete structure whilst those that show poor diffraction using XRD can be analysed at the Australian Synchrotron. Absolute configuration determinations are also possible through the application of the crystalline sponge method.[4] All compounds isolated with be evaluated at the CO-ADD and Nature Bank Australia for their potential therapeutic activity against a series of assays including an assessment of their antimicrobial activity.

References:
[1]. Newman D. J. and Cragg G. M. Journal of Natural Products **79** (2016) 629.
[2]. Farha M. A. and Brown E. C. Natural Product Reports **33** (2016) 668.
[3]. Brkljača R. and Urban S. Journal of Liquid Chromatography & Related Technologies **34** (2011) 2728.
[4]. Urban S. Brkljača, R., Hoshino, M., Lee, S. and Fujita, M. Angewandte. Chemie International Edition **55** (2016) 2678.

Contact Details:
To discuss this project further please contact:

Dr Sylvia Urban (sylvia.urban@rmit.edu.au) 1st Supervisor – 3.2.14
Dr Robert Brkljača (robert.brkljaca@rmit.edu.au) 2nd Supervisor – 3.1.005

Natural Product Studies of Australian Marine and Terrestrial Organisms – therapeutic potential

Applied Chemistry and Environmental Science Discipline/(Marine and Terrestial Natural Product (MATNAP) Research Group) – RMIT City

Project Description

Natural products continue to represent an important source for the search of therapeutic drugs. In the period 2000-2010, approximately 50% of all new drugs from this period have been either sourced directly or derived from natural product pharmacophores.[1] The proposed research will involve the extraction of selected marine and terrestrial organisms with the aim of isolating bioactive secondary metabolites. Any natural product isolated will be subjected to a complete structure characterisation as well as to biological activity evaluation. Column chromatography and HPLC will be the primary means of isolation and purification whilst NMR spectroscopy and mass spectrometry will be the two principle techniques used for structure characterisation and confirmation. HPLC-NMR will also be implemented to conduct chemical profiling studies that will expedite the discovery of new chemical entities.[2-3]

The targeted organisms will be extracted using organic solvents, and the compounds present will be separated on the basis of polarity using solvent partitioning. Isolation and purification will be achieved primarily through column chromatography and HPLC. Separated fractions will then be evaluated by analytical HPLC and ^{1}H NMR spectroscopy. Purified compounds will have their structure characterised and elucidated using 1D and 2D NMR spectroscopic techniques together with mass spectrometry. New compounds identified will be further characterised using UV and IR spectroscopy along with optical rotation measurements. Through existing collaborations with The University of Melbourne compounds that provide stable crystal structures can be analysed via X-Ray Diffraction (XRD) to obtain a complete structure whilst those that show poor diffraction using XRD can be analysed at the Australian Synchrotron. Absolute configuration determinations are also possible through the application of the crystalline sponge method.[4] All isolated compounds, once characterised, will have their antimicrobial activity assessed by a collaborator, the Community for Open Antimicrobial Drug Discovery (CO-ADD). The compounds will be tested against seven microorganisms, including methicillin-resistant *Staphylococcus aureus*. Further assessment of the therapeutic potential of isolated natural products will be assessed at Nature Bank Australia.

References:
[1]. Newman D. J. and Cragg G. M. Journal of Natural Products **79** (2016) 629.
[2]. Brkljača R. Göker E. and Urban S. Marine Drugs **13** (2015) 2714.
[3]. Brkljača R. and Urban S. Photochemistry **117** (2015) 200.
[4]. Urban S. Brkljača, R., Hoshino, M., Lee, S. and Fujita, M. Angewandte. Chemie International Edition **55** (2016) 2678.

Contact Details:
To discuss this project further please contact:

Dr Sylvia Urban (sylvia.urban@rmit.edu.au) 1st Supervisor – 3.2.14
Dr Robert Brkljača (robert.brkljaca@rmit.edu.au) 2nd Supervisor – 3.1.005

Bioactivity guided evaluation of the chemical components of indigenous Australian plants and an assessment of their suitability as potential lead therapeutic compounds

Applied Chemistry and Environmental Science Discipline/(Marine and Terrestial Natural Product (MATNAP) Research Group) – RMIT City

Project Description

The indigenous people of Australia are one of the oldest existent societies on the planet and their experience with the native flora of Australia spans tens of thousands of years. So far only a small fraction of the traditional medicinal repertoire has been screened. With Australia being classified as one of seventeen mega diverse countries on Earth, the biodiversity is high and the potential for discovering promising unknown pharmacophores is high.[1,2] The aim of this study will be to work with targeted plant species traditionally utilised by the Australian Aborigines, which can be sourced via a number of means (plant permits, access to indigenous nurseries or via research collaborations), and to let their biological activity guide which components and fractions of the specimen will be prioritized for further study. The overall aim will be to isolate bioactive secondary metabolites and all natural products isolated will be subjected to a complete structure characterisation as well as to biological activity evaluation. HPLC-NMR may also be implemented to conduct chemical profiling studies that will expedite the discovery of new chemical entities.[3]

The targeted plants will be extracted using organic solvents, and the compounds present will be separated on the basis of polarity using solvent partitioning. Isolation and purification will be achieved primarily through column chromatography and HPLC. Separated fractions will then be evaluated by analytical HPLC and ^{1}H NMR spectroscopy. Purified compounds will have their structure characterised and elucidated using 1D and 2D NMR spectroscopic techniques together with mass spectrometry. Through existing collaborations with The University of Melbourne compounds that provide stable crystal structures can be analysed via X-Ray Diffraction (XRD) to obtain a complete structure whilst those that show poor diffraction using XRD can be analysed at the Australian Synchrotron. Absolute configuration determinations are also possible through the application of the crystalline sponge method.[4] All isolated compounds, once characterised, will have their antimicrobial activity assessed by a collaborator, the Community for Open Antimicrobial Drug Discovery (CO-ADD). The compounds will be tested against seven microorganisms, including methicillin-resistant *Staphylococcus aureus*. Further assessment of the therapeutic potential of isolated natural products will be assessed at Nature Bank Australia.

References:

[1]. Crisp M. D. et al. Journal of Biogeography **28** (2001) 183.
[2]. Brkljača R. and Urban S. Journal of Natural Products **78** (2015) 1486.
[3]. Brkljača R. and Urban S. Photochemistry **117** (2015) 200.
[4]. Urban S. Brkljača, R., Hoshino, M., Lee, S. and Fujita, M. Angewandte. Chemie International Edition **55** (2016) 2678.

Contact Details:
To discuss this project further please contact:

Dr Sylvia Urban (sylvia.urban@rmit.edu.au) 1st Supervisor – 3.2.14
Dr Robert Brkljača (robert.brkljaca@rmit.edu.au) 2nd Supervisor – 3.1.005

DR229 – PhD (Applied Chemistry)
MR229 – Master of Science (Applied Chemistry)

School of Science HDR Project 2018

Functional Nanocrystal Inks for Printed Inorganic Solar Cells

Applied Chemistry and Environmental Science Discplline/ Nanostructure Laboratory - City Campus

Project Description:

One of the most attractive applications for solution-processed semiconductors is in the field of solar cells [1]. At present, the manufacturing of solar panels involves expensive high temperature and high vacuum processes. In order to mitigate these costs, and ultimately drop the cost of solar panels, considerable effort is currently being applied to the production of solar panels made from solution processed methods, which are amenable to high throughput, low cost, roll-to-roll printing techniques. The ability to simply print a solar cell in air at mild temperatures is unparalleled in its capacity to revolutionize solar cell manufacturing.

Innovative nanoscience will be used to develop "solar inks" composed of semiconductor nanocrystals. Nanocrystals provide an ideal means to generate semiconductor layers from solution wherein the nanocrystals act as a *template* for the formation of the desired microcrystalline semiconductor [2]. These nanocrystal templates can be synthesised cheaply and on large scales [3]. Furthermore, the exchangeable surface chemistry of nanocrystals permits them to be dispersed in a variety of solvents that are desirable for printing applications. In spite of their clear potential, at present these nanocrystal inks remain seriously underdeveloped.

The formulation and transformation of these inks into efficient semiconductor light absorbing layers and their incorporation into solar cells will be the key focus of this PhD project [4]. This project focuses on the light absorbing semiconductor material Cu_2ZnSnS_4 (CZTS) as it possesses excellent optoelectronic properties relevant to solar cells and is comprised of inexpensive, low toxicity, earth abundant elements [5]. This project will focus on *how* to improve the quality of (CZTS) nanocrystal "solar ink" dispersions and *what* conditions and chemistries are beneficial to transform these inks into microcrystalline semiconductor films.

The PhD program is flexible but will involve the core activities of nanocrystals synthesis, surface modification steps (surface chemistry), thin film deposition and characterization, optimization of thin film properties using thermal treatment steps and chemical methods, as well as solar cell device fabrication and testing.

References:

[1]. Polman, A., et al., Science, 2016, **352** (6283), p. 307.
[2]. Zhou, H., et al., Energy & Environmental Science, 2013, **6**, p. 2822.
[3]. van Embden, J., et al., Chemistry of Materials, 2015, **27**: p. 2246.
[4]. van Embden, J., et al., Journal of the American Chemical Society, 2014, **136**: p. 5237.
[5]. Chesman, A.S.R. and van Embden, J., et al., Crystal Growth & Design, 2013. **13**: p. 1720.

Contact Details:
To discuss this project further please contact:

Dr. Joel van Embden (joel.vanembden@rmit.edu.au)
Senior Supervisor
Kernot Building, Office 3.2.07

Synthesis of Novel Semiconductor Materials for Thin Film Optoelectronics

Applied Chemistry and Environmental Science Discipline Nanostructure Laboratory – RMIT City

Project Description:

A new paradigm has recently emerged in the form of solution-processed semiconductor-based devices.[1] The ability to achieve a pure solid semiconductor film using solution processed methods will accelerate breakthroughs in optoelectronic devices, such as phototransistors, light emitting diodes, photosensors, and solar cells.

This project focuses on a largely unexplored class of semiconducting materials from the pnictogen family. Antimony (Sb) and bismuth (Bi) containing semiconductors, such as (Sb_2Se_3, Cu_3SbS_4, $CuSbS_2$, $AgBiS_2$, and BiI_3), are extremely attractive as light-absorbing materials for photodetector and photovoltaic applications due to their large absorption coefficients and high charge carrier mobilities. [2,3] In addition to having the appropriate optical and electrical properties most Sb and Bi containing compounds also have very low melting points. This gives them a unique advantage over more established semiconductors such as c-Si, CdTe, CZTS, and CIGS, in that they may be processed into highly crystalline thin films at low temperatures.

Despite these attractive properties, research into Sb– and Bi– based semiconductors is still in its infancy. This project will address the need for detailed investigations into novel Sb– and Bi– based compounds, (specifically those containing halogen anions) and for their development into high quality thin films. This project has the scope for using multiple routes to generate the solar cell absorber layer. Solution-based methods such as nanocrystal templates [2,3] or inorganic–organic molecular precursors [4] are attractive and viable techniques. However, the facilities to explore evaporative techniques such as the Rapid Thermal Processing of semiconductor powders [5] (analogous to close space sublimation), is also available and encouraged.

The PhD program is flexible but will involve the core activities of novel material exploration and synthesis, optimization of thin film deposition techniques, as well as the optical and structural characterization of thin films. This project will also involve the testing and assessment of the fabricated thin films through their incorporation into solar cell devices.

References:

[1]. Polman, A., et al., Science, 2016, **352** (6283), p. 307.
[2]. van Embden, J. et al., Journal of the American Chemical Society 2013, **135**, p. 11562.
[3]. Bernechea, M. et al., Nature Photonics, 2016, **10**, p. 521.
[4]. Choi, Y. C. and Seok, S., et al,. Advanced Functional Materials, 2015, **25**, p. 2892.
[5]. Zhou, Y. et al,. Nature Photonics, 2015, **9**, p. 409.

Contact Details:

To discuss this project further please contact:
Dr. Joel van Embden (joel.vanembden@rmit.edu.au)
Senior Supervisor
Kernot Building, Office 3.2.07

Solution-Processed Scalable Perovskite Solar Cells Using a Mini-Reactor

Applied Chemistry and Environmental Science Discipline/ Nanostructure Laboratory -RMIT City

Project Description:

The emergence of hybrid organic–inorganic perovskite solar cells ($CH_3NH_3PbI_3$) has revolutionized the landscape of solar cell research. The efficiencies of perovskite solar cells have risen faster than any other solar cell technology in history. Their efficiencies have soared from 4% in 2009 to 21% at the end of 2016 [1]. They are currently considered the as the material to challenge the marketplace dominance of silicon [2]. To date, great effort has been put into improving both the precise perovskite composition and deposition parameters in order to achieve such high efficiencies [3]. However, many challenges surrounding device architecture, stability, and lifetime still need to be solved. In addition to solving these problems one of the major scientific challenges to the implementation of this technology at a commercial scale is the ability to reliably (and reproducibly) fabricate high quality perovskite thin films on large areas.

Existing methods to produce perovskite thin films rely on spin coating techniques (anti-solvent dripping [4] or gas-assisted quenching [5]) that are inherently unreliable and irreproducible, wherein large variations in film quality occur from batch-to-batch and for different experimentalists. Furthermore, spin coating techniques are only able to make devices on small scales. To address this problem, in this project a custom-built thin film "mini-reactor" will be used to produce the perovskite solar absorber layer. The novel deposition technique used by this reactor encourages the growth of highly crystalline thin films with large domain sizes in a reproducible manner. Importantly, the reactor design ultimately permits the direct scale-up of the film dimensions by simply increasing the size of the reactor.

The PhD program is flexible but will involve the core activity of optimizing perovskite thin film deposition using the novel mini-reactor. The scope includes optimization of the perovskite precursor solutions (composition, solvent, concentration etc.), investigations into the most applicable substrate layers (layers upon which the perovskite is deposited), modification of reactor function and design (as required), as well as solar cell device fabrication and testing.

References:

[1]. Bi, D., et al., Nature Energy, 2016, **1** (16142), p. 1.
[2]. Polman, A., et al., Science, 2016, **352** (6283), p. 307.
[3]. Stranks, S. D., Snaith, H. J., et al., Angewandte, 2015, **54**, p. 3240.
[4]. Li, X., Grätzel, M., et al., Science, 2016, 10.1126/science.aaf8060
[5]. Huang, F., et al., Nano Energy, 2014. **10**, p. 10.

Contact Details:

To discuss this project further please contact:

Dr. Joel van Embden (joel.vanembden@rmit.edu.au)
Senior Supervisor
Kernot Building, Office 3.2.07