DCU research project proposals for Notre Dame interns – January 2016

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Biomarker discovery in hybrid parasite genomes

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Project Aims

Leishmania are protozoan parasites transmitted by sandflies causing the neglected tropical disease leishmaniasis that infects 12 million people in over 98 countries. There are few molecular tools for monitoring the emergence of new *Leishmania* outbreaks, even though hybrids are formed frequently between species. The Infection Genomics laboratory at the DCU School of Biotechnology has used DNA from leishmaniasis infections to assemble genome sequences for three new species. We can now use these genome sequences to detect other inter-species infections by designing diagnostic tests for specific biomarkers. These molecular markers are sections of the DNA in genes that can be assessed to distinguish between different samples. Investigating the structure of potential biomarker genes and designing methods for their amplification is a crucial task for controlling parasitic disease.

Research Group and Techniques

The Nutritional Genomics and Infection Genomics laboratories at the School of Biotechnology in DCU has two faculty members, one postdoc, four PhD students, and another starting in 2016. To facilitate this project twinning molecular data with computational methods, the labs are equipped with a Dell PowerEdge computer server and a licence for using servers at the Irish Centre for High-End Computing. The student will be provided with specific training in homology searches, sequence alignments and database searches so that they can assess potential biomarkers using these methods. The student will learn about microbial evolution, molecular diagnostics and how to compare genomes.

Potential Candidates

This project would suit a motivated student who has interest in molecular and computational biology. The project involves skills such as DNA sequence comparison, visualising genomic data and computer programming: appropriate training will be provided. At the end of the project, you will be able to perform sequence alignments between genomes and interpret the effects on inferred gene models. Learning about these techniques is valuable for any student interested in bioinformatics or biomedical research on genomic data.

References

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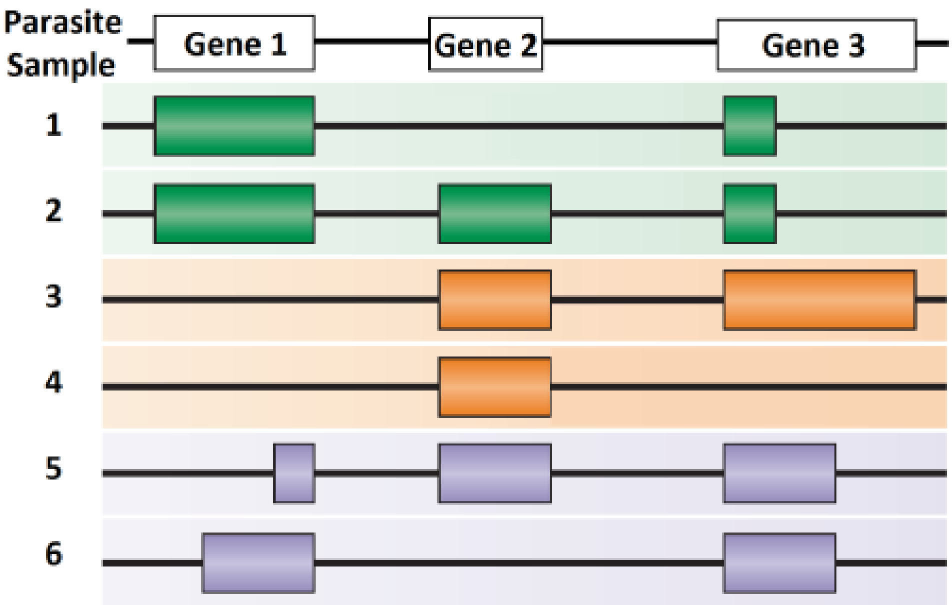

A study to examine dendritic cell-mast cell cross talk and the influence on adaptive immunity.

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Project aims and objectives

Dendritic cells (DCs) have a central role among innate immune cells in presenting antigen and priming T cells to differentiate into Th1/Th17 or Th2/Treg subsets. These cells express surface molecules and produce cytokines that modulate the effector functions of responding T-cells. While much is known of how these antigen presenting cells communicate with cells of adaptive immunity little is understood about how these cells communicate with other innate immune cells such as mast cells (MCs). To identify the underlying mechanisms of the immunoregulatory capacity of MCs, you will investigate the impact of MCs activated by our antigens upon dendritic DC maturation and function. Dendritic cells maturation and function will be measured by examining cytokine secretion patterns (IL-6, IL-12p70, IL-10 and NO) by ELISA and cells surface marker expression (CD40, CD80, CD86) by flow cytometry. You will determine if MC-"primed" DCs can subsequently induced efficient T-cell proliferation and cytokine secretion. This study will be one of the first to shed light on Mast cell-DC communication in this context.

Research Group

The Fundamental and Translational Immunology group, led by Dr Sandra O Neill, studies the innate and adaptive immune response during helminth infection, and its suppressive effects on allergenic and Th1/Th17 driven inflammatory processes. The group's research particularly focusses on understanding crosstalk between innate immune cells such as dendritic cells, mast cells and macrophage and their role in driving Th2, regulatory and anergenic T-cells. Another aspect of the research looks at the therapeutic benefits of helminth derived native and recombinant molecules. Understanding how these molecules interact with innate and adaptive immune cells, will identity new mechanisms to control inflammatory processes that could be exploited as novel therapeutics for inflammatory diseases and also as vaccine candidates to prevent helminth infection.

Potential Candidates

The project is ideal for a student who is interested in Immunology and cell biology. The project involves a number of skills such as culturing of primary cells from bone marrow, bioassays, PCR and flow cytometry. The candidate should be able to work with a team and will be expected following initial training by experienced post-doctoral scientist to work independently.

References

1. Adams PN, Aldridge AM, Vukman KV and O'Neill SM (2014) Fasciola hepatica tegumental antigens indirectly induce an M2 macrophage-like phenotype *in vivo*. Parasite Immunology, Oct;36(10):531-9.
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3. Vukman KV, Adams PN, Metz M, Maurer M, **O'Neill SM**. (2013) *Fasciola hepatica* tegumental coat impairs mast cells' ability to drive Th1 immune responses. J Immunol. 2013 Mar 15;190(6):2873-9.

Title: Marine-inspired materials for the prevention of biofouling on surfaces

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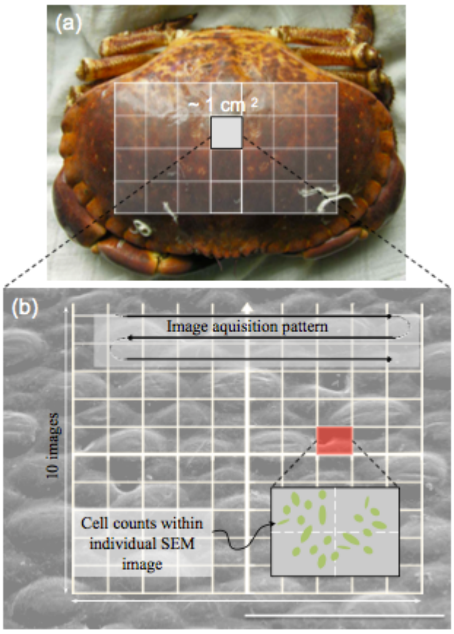
Project aims/Objectives

The marine environment is rich with species that have natural antifouling characteristics. This project will investigate the nature of surface texture on fish and shellfish using light microscopy and scanning electron microscopy (SEM). The features on fish surfaces will be studied in detail and the information will lead to the design of materials or coatings for application in the marine environment. [1-4] The figure opposite shows a scan pattern utilised for producing an image montage of a larger surface area from the carapace of C. pagurus (brown crab) [1] using SEM. These studies will be carried out on fish caught in Irish waters.



Research group/Techniques

This work will form part of a group of projects looking at materials for antifouling coatings. The group currently has three postdoctoral researchers and 5 graduate students. The student will have access to a range of specialist instrumental techniques (spectroscopy, imaging) as well as routine analytical and deployment techniques (laboratory tanks or marine structures) including algal cultures for in-lab testing of materials.

Potential Candidates

This project would suit a student with an interest in environmental science, material science and engineering, marine science, analytical science. The project will involve skills of microscopy (SEM, confocal), image analysis, materials development using polymer synthesis, sample testing using diatom (algae) cultures and biochemical assays. The candidate will be supported by two researchers in the group at all times, one on material development and testing and a second on species characterization.

References

1. Sullivan, Timothy; Mcguinness, Kevin; O Connor, Noel; Regan, Fiona. , Characterisation and anti-settlement aspects of surface micro-structures from Cancer pagurus, Bioinspir Biomim. 2014 Oct 7;9(4):046003. doi: 10.1088/1748-3182/9/4/046003.
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3. James Chapman, Tim Sullivan, Eolann Kitteringham, Fiona Regan, Antifouling Performances of Macro- to Micro- to Nano- Copper materials for the Inhibition of Biofouling in its Early Stages, Journal of Materials Chemistry B. 2013,1, 6194-6200
4. James Chapman, Claire Hellio, Tim Sullivan and Fiona Regan, Bioinspired synthetic macroalgae: examples from nature for antifouling applications, International Biodeterioration & Biodegradation, Volume 86, Part A, 2014, Pages 6-13.

Title: The removal of organic pollutants from contaminated compost to produce commercially viable materials for sale.

Dr. Brian Kelleher (Brian.Kelleher@dcu.ie)

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Organic pollutants in soil and compost such as aromatic hydrocarbons, polycyclic aromatic hydrocarbons (PAH's) and polychlorinated biphenyls (PCBs) threaten soil and water supplies and therefore public health. They are ubiquitous environmental pollutants and many are known carcinogens and mutagens. Reducing the level of organic pollutants eliminates one of the factors preventing mixed waste composted material from being used as an agricultural fertiliser. The Environmental Protection Agency Waste Report 2011* estimates that 720,000 tonnes of biodegradable waste are generated each year in Ireland. This has the potential to create 300,000 tonnes of compost. Eliminating organic pollutants from this material means it could be used to replace up to 60,000 tonnes of imported synthetic fertilizer whose current average import price is circa €400 per tonne. In this project we couple state-of-the-art microbiological and chemical analytical techniques to identify optimum conditions for the microbial breakdown of pollutants in these potentially valuable materials.

An internship would contribute to the following objectives:

- To develop chemical and microbiological techniques for the identification of organic pollutants such as aromatic hydrocarbons and poly aromatic hydrocarbons (PAHs) in compost and at different stages in the composting process.
- To identify the parameters that influence the rate of destruction of organic pollutants in composting.
- To identify specific microorganisms that will degrade targeted organic pollutants.
- To explore the possibility of cultivating such specific microorganisms for augmentation of the composting process.

It is envisaged that the successful student will assist in sampling and chemical/physical analysis of the composting experiments and if interested, could develop their own side project in collaboration with supervisors/colleagues.

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Modelling growth of ZnO nanowires – effects of wire shadowing on growth

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ZnO is a promising semiconducting material with many exciting applications and a strong propensity to grow in nanostructured form. ZnO nanostructures display a wide range of morphologies which are sensitive to growth parameters such as temperature, substrate type and the method used to generate source species [1]. Because of this sensitivity and morphological diversity, a greater theoretical understanding of the growth process is required in order to reproducibly grow specific ZnO nanostructure morphologies, especially on an industrial scale.

Our group has undertaken a number of theoretical/ computational studies of ZnO nanowire growth via the Vapour Phase Transport (VPT) growth method and reasonable overall agreement between theory and experiment has been found, e.g. in terms of average nanowire properties such as length, diameter etc. [2-4]. However, experimental results also show a substantial degree of scatter in physical quantities such as nanowire lengths [4] and the origin of this scatter is at present still unclear.

One physically plausible possibility is that the scatter in nanowire lengths is related to shadowing effects/competition for available source material amongst closely spaced nanowires and some experimental data support this hypothesis [4]. The summer intern project proposed here is to develop a theoretical/computational model and to test this hypothesis, building on the existing studies performed in our group and adding to these by incorporating the effects of shadowing/competition into those models, e.g. perhaps by Monte-Carlo techniques.

This summer intern project would suit a physics, engineering, materials science or physical chemistry student with an interest in nanoscience and an interest and ability in mathematics and computational science.

Further details can be obtained by contacting Dr. Enda McGlynn by email, at the email address given above.

[1] Z.L. Wang, Zinc oxide nanostructures: growth, properties and applications, Journal of Physics: Condensed Matter, 16 (2004) R829–R858.

[2] R.B. Saunders, E. McGlynn, M. Biswas, M.O. Henry, Thermodynamic Aspects of the Gas Atmosphere & Growth Mechanism in Carbothermal Vapour Phase Transport Synthesis of ZnO Nanostructures, Thin Solid Films, 518 (2010) 4578–4581.

[3] R.B. Saunders, E. McGlynn, M.O. Henry, Theoretical Analysis of Nucleation and Growth of ZnO Nanostructures in Vapour Phase Transport Growth, Crystal Growth and Design, 11 (2011) 4581–4587.

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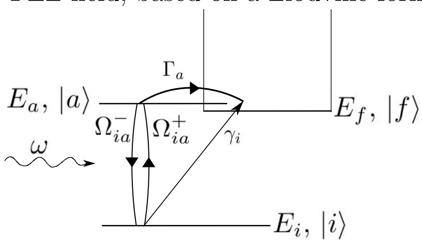
Stochastic Rabi dynamics of atoms under FEL radiation

Motivation: 20th century's X-ray radiation was proven of great importance across a number of research areas from physics, chemistry, biology and medicine sciences. 21st century's revolutionary free-electron laser (FEL) technological breakthroughs have resulted to the production of intense, ultrashort and coherent X-rays. The availability of radiation with such properties (not present in synchrotron radiation) allows *for the first time* the real-time tracking of the internal dynamics of nanoscale-size systems, ranging from small quantum systems to large biological structures. Despite these unique properties, at its current stage, the FEL radiation field $\mathcal{E}(\mathbf{r}, t)$ experiences strong amplitude and phase *random* fluctuations. Consequently, in certain cases, the interpretation of the physical processes that involve the interaction of the FEL radiation with matter, neccessitates to take the stochastic component into account. The latter requirement represents the motivation of the current proposal.
Project: *The investigation of the effects of the stochastic fluctuations of an x-ray FEL field of central frequency* ω *on the resonant excitation* ($|a\rangle$) *and ionization* ($|f\rangle$) *dynamics of the innermost 1s-shell electron of the neutral neon* ($|i\rangle$) *(see figure and Ref [1]).*
Method: As stochastic phenomena are characterized by their coherence properties we'll derive the stochastic density matrix state ($\hat{\rho}(t)$) equations that govern the interaction of the neon with the FEL field, based on a Liouville formulation,



$$\imath \frac{d}{dt}\hat{\rho}(t) = [\hat{H}(t), \hat{\rho}(t)], \quad \hat{H}(t) = \hat{H}_0 - \mathbf{r} \cdot \mathcal{E}(t),$$

where $\hat{H}_0$ is the field-free neon atomic Hamiltonian. The stochastic variations of the field will be modelled as a *Gaussian*, *stationary* stochastic process. The assumption of stationarity simplifies considerably the mathematical aspects of the problem and an ensemble averaging technique can be followed. This method avoids the use of the straightforward, but computationally demanding, Monte Carlo technique. It is worth noting that, in viewing the Liouville equations as a system of differential equations, the present formulation is equivalent to stochastic problems that frequently appear in risk analysis of finance market (*econophysics*).
Outcomes: In formulating the stochastic Liouville equations for the present project, the student:

1. Will come into contact with the practicalities of Liouville equation in terms of the system's state density matrix ($\imath\dot{\hat{\rho}}(t) = [\hat{H}(t), \hat{\rho}(t)]$) as an alternative of the Schrödinger's equation description in terms of the system's state wavefunction ($\imath\partial_t\psi(t) = \hat{H}(t)\psi(t)$).

2. Will come into contact with methods of solving stochastic differential equations.

3. Will extend a code, developed from a previous Naughton fellow [2], to include a proper 1st/2nd-order coherence function for a realistic FEL radiation. Quantitative comparisons with the results of Ref. [1] (calculated through a Monte-Carlo approach) will be performed to demonstrate the efficiency and reliability of the present ensemble-averaging method.

Skills required: A basic knowledge of the quantum mechanics concepts, and familiarity with one of the standard programming languages (e.g. f77/f90/C++/C) and the UNIX/Linux/Mac OSX operating systems. The project is suited for students with strong interest in the theoretical/computational aspects of AMO (atomic,molecular & optical), photonic and nanosystems physics.
References:
[1] Nina Rohringer and Robin Santra, Phys. Rev. A **77**, 053404 (2008).
[2] Sean Howard, Naughton REU report (2014), (unpublished).
Project supervisor:
Dr. Lampros Nikolopoulos, e-mail:Lampros.Nikolopoulos@dcu.ie

Resonant Laser Induced Breakdown Spectroscopy (R-LIBS) for the Classification and Quantification of Key Elements in Steel

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Project Aims/Objectives

Laser Induced Breakdown Spectroscopy (LIBS) is a standard approach for classifying materials be they solid, liquid or gas [1]. LIBS involves using a laser to create an ionized vapour on the surface of a large sample to create a plasma. The spectrum of light emitted from the plasma is characteristic of the elemental composition of the sample, effectively a chemical fingerprint. The properties of steel depend on the presence of other elements such as carbon, sulphur, manganese, etc present even at very low concentations. Here we will use LIBS to determine the presence of elements in steel [2]. The wavelength of the light will be chosen to correspond to a resonance of a known element within the solid sample which we expect to lead to a much improved limit-of-detection (LOD). The tunable wavelength will be provided by an Optical Parametric Oscillator (Contiuum Panther™). In addition to tuning the wavelength, if time permits, we will combine employ double pulse LIBS [3] to further optimise the LOD. For complex/rich spectra we will employ statistical techniques, especially Principal Component Analysis [4], for which we have a code now at an advanced stage of development by one of the group.

Research Group / Techniques.

The Laser Plasma and AMO at the School of Physics in DCU is well established in intense laser matter interactions. We have a suite of well-equipped laboratories, for a list of equipment – cf http://www.physics.dcu.ie/~jtc/expfacil.html. The group currently comprises 4 faculty members, 1 SFI Fellow, 3 postdoctoral fellows and 10 research students. Our high power lasers produce pulses from the femtosecond to nanosecond range and our spectrometers cover the NIR to soft X-ray range. As a member group of the National Centre for Plasma Science and Technology at DCU we also have access to many materials diagnostics like XRD, AFM, SEM, etc. We also have a number of codes for atomic spectra calculations to aid LIBS.

Potential Candidates

This project would suit a student who has interest in lasers, optics and spectroscopy. The project involves skills such as optical alignment, vacuum technology and data processing in MATLAB. The candidate should be comfortable working in a high power (Class IV) laser environment (appropriate training will be given and the student will be accompanied by an experienced research student and/or postdoc at all times).

References

[1] R. Noll, Laser-induced Breakdown Spectroscopy, Springer (2012)

[2] X Jiang, P Hayden, J T Costello and E T Kennedy, Dual-Pulse Laser Induced Breakdown Spectroscopy with Ambient Gas in the Vacuum Ultraviolet: Optimization of Parameters for Detection of Carbon and Sulphur in Steel
Spectrochimica Acta Part B: Atomic Spectroscopy **901** 106-113 (2014)

[3] M.A. Ismail, G. Cristoforetti, S. Legnaioli, L. Pardini, V. Palleschi, A. Salvetti, E. Tognoni, M.A. Harith, Comparison of detection limits, for two metallic matrices, of laser induced breakdown spectroscopy in the single and double-pulse configurations, *Anal. Bioanal. Chem.* **385** 316–325 (2006)

[4] S. M. Clegg, E. Sklute, M. D. Dyar, J. E. Barefield and R. C. Wiens Multivariate analysis of remote laser-induced breakdown spectroscopy spectra using partial least squares, principal component analysis, and related techniques *Spectrochimica Acta Part B* **64** 79–88 (2009)