

# **NSF GROW – Potential Research Hosts in Ireland**

## **US-Ireland Awardees**

## Principal Investigator

**Prof Debra F. Laefer**

**Prof John O'Sullivan**

Email: [debra.laefer@nyu.edu](mailto:debra.laefer@nyu.edu); [jj.osullivan@ucd.ie](mailto:jj.osullivan@ucd.ie)

Website:

<https://wp.nyu.edu/urbanmodeling/>

## Host Institution

University College Dublin

## Project Title: AMASS: Advanced Manufacturing for the Assembly of Structural Steel

### *Research Programme Description*

The structural performance of a new steel connection will be studied and gradually improved through a series of tests and numerical modelling. Small-scale testing will be conducted at UCD. The tests will explore the connection's structural behaviour, initially under simple load conditions and later under complex ones. The information gained from the tests will be used to improve the numerical model for multi-interface, steel-to-steel connection and to refine the geometric connection arrangement. Novel visualization techniques will be applied using multiple, high frame rate cameras, and Structure from Motion visualization techniques to try to gain further insights into the deformation and failure mechanisms.

The tested samples will be fabricated using the best connection details obtained from previous numerical and test results. Test reports with load-deflection, moment-curvature, and failure loads and 3D printed models from SfM techniques

The program activities involve:

- Preparing the tested beam drawings
- Contacting the steel fabricator and arranging for them to be fabricated
- Preparing the experimental setup
- Calibrating the loading machine required to conduct beam testing
- Upon delivery of the beams:
  - Instrumenting the test models
  - Carrying out the test
  - Analysing the results and preparing test reports

## Principal Investigator

**Prof. Luiz DaSilva** ([dasilval@tcd.ie](mailto:dasilval@tcd.ie))

**Prof. Nicola Marchetti** ([nicola.marchetti@tcd.ie](mailto:nicola.marchetti@tcd.ie))

**Dr. Jacek Kibiłda** ([kibildj@tcd.ie](mailto:kibildj@tcd.ie))

### Website:

CONNECT Research Centre, Trinity College Dublin:

<https://connectcentre.ie>

**Prof. DaSilva's website:** <https://luizdasilva.wordpress.com>

### *Host Institution*

Trinity College Dublin

***Project Title: When mobile networks ride the millimetre-waves:  
managing wireless resources in cross-frequency 5G networks***

### *Research Programme Description*

The NEMO project – Enabling Cellular Networks Exploit Millimetre-wave Opportunities - brings together researchers at Trinity College Dublin, Queen's University Belfast, and Virginia Tech, to design the integration of mmwave technology in large mobile networks. We combine expertise on propagation models, experimentation, and mathematical analysis of wireless networks, in the three institutions to develop a complete vision of how this new technology will enable the next generation of wireless services, from self-driving cars to haptic Internet to augmented reality.

A lesson from the research we conducted so far is that mmwave links are much more unpredictable than the conventional sub-6 GHz links. This is due to the peculiar characteristics of the physics of mmwave propagation, which is highly impacted by the the high absorption by obstacles, weak scattering and diffraction, or severe power fades due to micromobility. The objective of this project is to explore the statistical properties of these mmwave uncertainties, relative to the properties of the uncertainty models for conventional cellular links, aiming at determining the cross-tier resource management strategies to be employed by the network to achieve service-level robustness and reliability.

The NSF Graduate Research Fellow will collaborate with our group in one or more of the following tasks:

1. Build a statistical framework to describe said uncertainties;
2. Propose a set of resource management scenarios, which will guide channel measurement campaigns conducted in collaboration with our partners at Queen's University Belfast;
3. Use the developed analytical framework informed by the empirical results from the channel measurements, to design resource management mechanisms for cross-tier mobile networks;
4. Apply game theory to design improved resource management mechanisms in cross-tier networks, which are efficient, fair and stable over time.

## Principal Investigator

**Prof Liam Barry**

Email: [liam.barry@dcu.ie](mailto:liam.barry@dcu.ie)

**Website:** <http://www.eeng.dcu.ie/~barry/>

## Host Institution

Dublin City University

## Project Title: Characterisation of wavelength tuneable lasers for reconfigurable optical networks

### *Research Programme Description*

The desire for multi-media content and richly interactive data services is shaping a new era for communications networks. Future networks will need to be capable of offering Triple Play, IPTV, Video-on-Demand, Voice-over-IP and High-Speed Internet Access, combined with guaranteed Quality of Service. These networks will employ wavelength division multiplexing (WDM) technology, and advanced modulation formats, in order to achieve the high capacities required. In addition, given the bursty nature of this data it is expected that dynamic allocation of the bandwidth will be implemented to efficiently use the available capacity. The key component in these networks will be the tuneable laser transmitters that generate the different wavelength packets. This research programme will explore novel applications and implementations of wavelength tuneable lasers in optical WDM metro, access, and datacentre networks. Specifically, we will investigate (i) direct modulation of tuneable lasers, (ii) use of advanced modulation formats and OFDM in fast reconfigurable networks, and (iii) development demonstrations of low cost high capacity systems. The research will span device and system design, numerical modelling, experimental characterisation, and system evaluation using the wide-ranging research capabilities of the laboratory facilities in Dublin City University

## Principal Investigator

**Dr Eugene O'Brien**

Email: [eugene.obrien@ucd.ie](mailto:eugene.obrien@ucd.ie)

### Website:

<http://www.ucd.ie/research/people/civilengineering/professoreugeneo'brien/>

## Host Institution

University College Dublin

## Project Title: Bridge Health Monitoring using Cameras and Other Sensors

### *Research Programme Description*

Deteriorating bridges have become a major societal concern, especially in the developed countries. The goal of this project is to explore computer vision algorithms and technologies, along with structural health monitoring methods, to develop an accurate, practical and low-cost bridge monitoring system that can identify any reduction in bridge safety in an objective and timely manner. The engineering challenges are global.

Today, most bridges are inspected manually, i.e., a person **looks** at the bridge to check for signs of deterioration. The results are inconsistent between inspectors and highly subjective. What is needed is a method of electronic monitoring using sensors to determine when a bridge is safe. We have been working with cameras with two objectives in mind: (1) to use cameras to measure bridge deflection and (2) to use other cameras to identify the vehicle(s) causing that deflection. We have also been using other sensors such as accelerometers mounted on the bridge or mounted in vehicles passing over the bridge. The latter is known as 'drive by' bridge inspection and is really promising as it would save a great deal of money if every bridge in the network could be checked in the length of time it takes to drive around the network. Apart from monitoring the bridge to look for signs of damage, we are monitoring bridge traffic loading. This is a statistical problem – we need to identify the probability of a critically dangerous traffic loading scenario being on the bridge during its lifetime. Further details by email or skype (ejobrien1).

## Principal Investigator

**Dr Niall Barron**

Email: [niall.barron@dcu.ie](mailto:niall.barron@dcu.ie)

Website: <http://nicb.ie/team-view/dr-niall-barron/>

**Dr Sandra Roche**

Email: [sandra.roche@dcu.ie](mailto:sandra.roche@dcu.ie)

Website: <http://nicb.ie/portfolio-view/pancreatic-cancer/>

## Host Institution

National Institute for Cellular Biotechnology, Dublin City University

## Project Title: Optimisation of chemotherapy regimes in pancreatic cancer using patient-derived xenograft (PDX) models

### *Research Programme Description*

Pancreatic cancer is the fourth leading cause of cancer deaths. Currently for patients diagnosed with pancreatic cancer there is a 5-year survival rate of 7% in the Republic of Ireland. Pancreatic cancer remains one of the most difficult malignancies to treat, with a 9-month median survival rate for locally advanced and approximately a 6-month median survival rate for metastatic pancreatic cancer. Many facets contribute to the poor outcome demonstrated in the clinic, including stage at diagnosis, advancement of the disease locally and distant metastasis. However, perhaps the most crucial factor relates to the ineffectiveness of current treatment regimes.

Many chemotherapy options have been explored in pancreatic cancer treatment. A recent multi centred phase II/III trial compared FOLFIRINOX versus gemcitabine. FOLFIRINOX is a combination of four agents; 5-FU, Irinotecan, Oxaliplatin and Leucovorin. FOLFIRINOX is considered a standard treatment option for patients with advanced pancreatic cancer, who are physically robust enough to withstand the treatment.

Pancreatic cancer surgical resection is limited to two hospitals in the Rep. of Ireland, Cork University Hospital and St Vincent's University Hospital (SVUH), Dublin. Through collaboration with SVUH, our group initiated the first Irish national patient-derived xenograft (PDX) models of pancreatic cancer. By implanting freshly dissected, pathologically confirmed, pancreatic tumour material into SCID mice, we developed xenograft models for investigating pancreatic tumour development, progression and drug response. This unique resource has given rise to a bio-bank of patient-derived tumours, as well as a living repository. Using these tumours, a number of novel pancreatic cell lines have been developed.

Using these novel primary cell lines and established cell models we are examining FOLFIRINOX scheduling *in vitro* combined with *in silico* pharmacology modelling to determine optimum schedule to maximise efficacy and minimise toxicities.

## Principal Investigator

**Assoc Prof Brian Rodriguez**

Email: [brian.rodriquez@ucd.ie](mailto:brian.rodriquez@ucd.ie)

### Website:

<http://www.nanofunction.org/p/people2&c=24>

<http://www.ucd.ie/research/people/physics/assoc%20professorbrianrodriquez/>

## Host Institution

University College Dublin

## Project Title: Nanoscale Function Group

### *Research Programme Description*

We are a highly interdisciplinary group based in the Conway Institute of Biomolecular and Biomedical Research and the School of Physics at University College Dublin in Ireland with diverse research interests spanning:

- Functional bio-materials and bio-compatible materials for energy harvesting and bio-sensing applications
- Advanced scanning probe microscopy-based characterization of biological and energy-related materials
- Development of scanning probe microscopy tools for probing ion diffusion, electrochemistry, and catalysis in solution
- Cell migration assays based on aligned collagen matrices for tissue engineering and drug screening applications
- 3D bioprinting for tissue engineering applications
- Biosensing using ferroelectric lithography-defined plasmon-active metallic nanostructure arrays
- Axon guidance for neuronal repair

We currently have 1 postdoc and 6 PhD students in the group and a well-equipped lab with 8 atomic force microscopes and 6 3D printers.

## Principal Investigator

**Professor Mike Zaworotko**

Email: [michael.zaworotko@sspc.ie](mailto:michael.zaworotko@sspc.ie)

## Website:

<http://www.ul.ie/crystalengineering>

[www.sspc.ie](http://www.sspc.ie)

## Host Institution

Synthesis & Solid State Pharmaceutical Centre (SSPC), University of Limerick

## Project Title: Predictive Asymmetric Synthesis

### *Research Programme Description*

This research programme aims to develop new methodologies for the asymmetric synthesis of existing active pharmaceutical ingredients (APIs) and future drug candidates with particular focus on the discovery and application of enzymes, small molecule organocatalysts and organometallic complexes for industrially-relevant, synthetic transformations. Green chemistry approaches with the potential for application in flow chemistry will be investigated with some projects underpinned by computational and predictive modelling.

Example projects include:

- a. *Biocatalytic Approaches to Asymmetric Synthesis*
- b. *Organocatalytic Approaches to Asymmetric Synthesis*
- c. *Transition Metal-Catalysed Approaches to Asymmetric Synthesis*
- d. *Green and Flow Approaches for Synthesis*

The development and application of predictive modelling in collaboration with a modelling group will be an integral part of this research programme.



## Principal Investigator

**Professor Mike Zaworotko**

Email: [michael.zaworotko@sspc.ie](mailto:michael.zaworotko@sspc.ie)

## Website:

<http://www.ul.ie/crystalengineering>

[www.sspc.ie](http://www.sspc.ie)

## Host Institution

Synthesis & Solid State Pharmaceutical Centre (SSPC), University of Limerick

## Project Title: Crystalline Drug Substances for Improved Medicines

### *Research Programme Description*

The field of chemistry that studies the design, properties and applications of new crystalline materials, crystal engineering, has grown exponentially over the past 25 years largely because composition and structure profoundly impact the physicochemical properties of crystalline solids and can lead to new benchmarks in terms of properties. Examples of the successful application of crystal engineering are exemplified by ultramicroporous materials, which have afforded new benchmarks for gas adsorption of commodity gases such as CO<sub>2</sub> and ethylene, and cocrystals, that have addressed solubility and stability challenges in drug substances. Cocrystals are a type of MCCM (multi-component crystalline material), comprising two or more compounds (coformers) that, when pure, exist as a solid or low volatility liquid under ambient conditions. Whereas cocrystals are long-known in the scientific literature, they remain understudied, especially relative to their potential. This is likely because cocrystals are typically only accessible when stoichiometric quantities of each coformer are present in a crystallisation medium. That MCCMs, especially cocrystals, can dramatically change physicochemical properties without changing the molecular structure of a biologically active molecule, lies behind their relevance to pharmaceutical science. Indeed, pharmaceutical cocrystals, i.e. cocrystals comprising at least one biologically active compound, have recently emerged as an option for drug substances, primarily because the efficacy of drug molecules which suffer from low aqueous solubility can be improved.

Example projects in this programme include:

- a. *Rapid discovery of MCCMs with improved physicochemical properties,*
- b. *Determining how co-formers impact biological efficacy*
- c. *Molecular level understanding of excipient-drug substance interactions.*

The development and application of predictive modelling in collaboration with a modelling group will be an integral part of this research programme.

## Principal Investigator

**Professor Gavin Walker**

Email: [gavin.walker@sspc.ie](mailto:gavin.walker@sspc.ie)

## Website:

[www.bernalinstitute.com](http://www.bernalinstitute.com)

[www.sspc.ie](http://www.sspc.ie)

## Host Institution

Synthesis & Solid State Pharmaceutical Centre (SSPC), University of Limerick

## Project Title: Predicting and controlling the efficacy of drug products

### *Research Programme Description*

The overall programme objective is to optimise the development, production and use of safe and effective medicines focusing on poorly soluble drugs, personalized and age appropriate medicines and rational formulation approaches with predictive performance.

An example project would be “Optimisation and modelling of in vitro and in vivo performance of enabling formulations for poorly soluble drugs” with the objective to advance formulation options for BCS class II and IV drugs and develop predictive models (in vitro and in silico) to determine the behaviour of solid oral formulations of such drugs in vivo. Additional projects in this programme include a. Flexible manufacturing platforms and formulation approaches for personalised and age-appropriate medicines and b. Advanced material characterisation for solid dosage forms with a view to rational, predictive formulation design, both of which set out to elucidate the relationships between powder fundamental and derived properties, processability and product performance for a range of APIs and solid dosage formulations, both immediate release and modified release formulations.

The development and application of predictive modelling in collaboration with a modelling group will be an integral part of this research programme.

## Principal Investigator

**Professor Gavin Walker**

Email: [gavin.walker@sspc.ie](mailto:gavin.walker@sspc.ie)

## Website:

[www.bernalinstitute.com](http://www.bernalinstitute.com)

[www.sspc.ie](http://www.sspc.ie)

## Host Institution

Synthesis & Solid State Pharmaceutical Centre (SSPC), University of Limerick

## Project Title: Next Generation Pharmaceutical Manufacturing

### *Research Programme Description*

It is widely recognised that within the next decade there will be a disruptive change in how we manufacture drug substance (DS) and drug product (DP) at End-to-End levels. This will align to an Industry 4.0 approach in manufacturing and ultimately to a “Pharmaceuticals 4.0” approach by 2025. This research programme will focus on the development and implementation of Continuous Manufacturing (CM) techniques, Flow Chemistry and End-to-End manufacturing methodologies from DS to DP. Manufacturing (DS, DP and coupled DS-DP) in the future is likely to be ‘skid mounted’, agile and mobile, requiring this research programme to be truly multi-disciplinary, leading to innovation at the interfaces between chemistry, process engineering, data analytics and mathematical modelling. CM in particular offers low facility cost, flexible batch (supply chain flexibility), platform tech, better QA (not better quality), yield improvements, and decreased Technology Transfer effort. The research will also assist in enabling new strategies and promote innovation and continual improvement, strengthen QA and reliable supply of product, including proactive planning of supply chain adjustments. This will allow regulators (assessors and inspectors) to better understand firms’ Pharmaceutical Quality Systems for management of post-approval CMC changes. There will be focus on Process Modelling and PAT for model predictive control of pharmaceutical manufacturing and on modularisation and intensified manufacturing to support the requirement to perform smaller volume manufacturing in specific countries to achieve regulatory approval.

Example projects in this programme include:

- a. *Hybrid Processing and Automated Process Design*
- b. *Continuous and Miniaturised Manufacturing*
- c. *Advanced Manufacturing Techniques*

The development and application of predictive modelling in collaboration with a modelling group will be an integral part of this research programme.

## Principal Investigator

**Prof Dónal Leech**

Email: [Donal.leech@nuigalway.ie](mailto:Donal.leech@nuigalway.ie)

Website: <http://www.nuigalway.ie/our-research/people/chemistry/donalleech/>

## Host Institution

National University of Ireland Galway

## Project Title: Electrochemical Protein Biomarker Arrays

### *Research Programme Description*

The research programme seeks to discover if *detection of a small panel of biomarker proteins in patient serum can be used to accurately detect and establish the stage and grade of cancers*, with an initial focus on prostate cancer. The objectives of the project are to develop an optimized, validated biomarker panel and appropriate measurement arrays to help establish the grade and stage of cancer as well as to identify patients free of cancer. Development of the biomarker panel is achieved by evaluating an appropriate biomarker set combining general accepted biomarker proteins with newly identified biomarker proteins for grade and stage of cancer recently identified.

Development of assays and validation of the biomarker panel is achieved with a rapid, ultrasensitive, yet inexpensive, microfluidic immunoassay system that has already been developed at by a collaboration with the University of Connecticut (Prof. Jim Rusling). Improvement in the assay protocols is to be achieved, through identification of antibodies, optimization of amplification procedures (using nanostructured surfaces, magnetic particles loaded with enzyme labels, and design of improved redox mediators). Parallelization using microelectrode arrays is proposed to permit rapid screening of samples.