

# SUMMER FELLOWSHIP PROGRAMME 2024 PROJECT DESCRIPTIONS









## **TABLE OF CONTENTS**

01	BioPhotonics	03 - 15
02	Circuit Design	16
03	Emerging Materials & Devices  Materials Theory  Nanotechnology	17 - 27
	Adavnced Nano Sensors	
04	Energy	28 - 29
05	Integrated Sensors Life Science Interface Nanotechnology	30 - 32
06	Monolithic & Heterogeneous Integrations Photonics Theory III-V Materials	33 - 44
07	Optical Communications	45 - 50
80	Smart Systems	51 - 52
09	Wireless RF Communications	53 - 55

# Beam shaping for designing an effective optical probe to minimize polymer signals for assessing in-bag blood quality.

Theme: BioPhotonics Supervisor: Rekha Gautam

Co-Supervisor: Sanathana Konugolu Venkata Sekar



#### Background:

Blood transfusion is a lifesaving therapy and is used to treat diverse patient populations. According to WHO, -120 million blood donations are collected every year globally, however, many patients requiring transfusion do not have timely access to it owing to the short shelf life of the blood products. For instance, red blood cells (RBCs) are allowed to store only for up to 35 days at 2-6°C once drawn out of the body. RBCs storage is associated with changes in cell integrity, hemolysis, methemoglobin, lactate, and microvesicles (called 'storage lesions'). Transfusion with this mixture of 'storage lesions' may result in adverse outcomes in patients. At present, there is no method for assessing the quality of blood products without potentially compromising the sterility of the unit, and storage age is considered as a surrogate for the efficacy and safety of blood. However, the storage age neither is reliable to assume blood products are safe for transfusion nor to discard a rare/lifesaving blood product 1 2,3.

#### Methods:

This project aims to develop a non-invasive multimodal probe to assess the quality of blood products inside the bag without compromising the sterile conditions. Involving optical design and characterization for measuring resonance Raman spectra at 633 nm using different optical designs.

#### Experimental activities:

Development and characterization of the different input beams. Initially the system will be tested on polymer bag filled with haemoglobin/hemin solution. The student will be characterizing the system for its performance in terms of stability, reproducibility, signal to noise (SNR) and accuracy. Following characterization, validation of the system will be performed on expired blood-bags obtained from Irish Blood Transfusion Service, Cork.

Theoretical activities: Data analysis will involve some pre-processing including- baseline correction, normalization, exponential fitting, and simulations.

The student will be given training on the optical design/instrument building aspects of the resonance Raman system, a systematic procedure to characterize and validate the system and data analysis.

#### Predicted results and impact:

Currently there is no non-invasive method for examining storage lesions in-bag. The proposed spectroscopic methods can impact the practice of transfusion medicine by directly characterizing RBCs in-bag objectively. This will help in better inventory management, minimizing wastage, and potentially improving patient outcomes by allowing informed selection of units. Further, the scope of this research can be extended to other blood products, tissues, cells, organs used for transplantation.

#### References:

- Gautam R, Oh J-Y, Marques MB, Dluhy RA, Patel RP. Characterization of Storage-Induced Red Blood Cell Hemolysis Using Raman Spectroscopy. Laboratory Medicine. 2018;49(4):298-310. doi:10.1093/labmed/lmy018
- 2. Gautam R, Oh JY, Patel RP, Dluhy RA. Non-invasive analysis of stored red blood cells using diffuse resonance Raman spectroscopy. 10.1039/C8AN01135D. Analyst. Dec 3 2018;143(24):5950-5958. doi:10.1039/c8an01135d
- Carey PR. CHAPTER 5 Resonance Raman Studies of Natural, Protein-Bound Chromophores.
   Biochemical Applications of Raman and Resonance Raman Spectroscopes. Academic Press; 1982:99-153.

Location: Tyndall Type: In-person, Hybrid

Key words: Optical Instrument Design, Diffuse Optics, Resonance Enhancement, Raman Spectroscopy

Degree(s) that will suit this project: Optics, Physics, Physical Chemistry

### Diffuse reflectance spectroscoNpy (DRS) to assist quantification of Raman signals

Theme:

BioPhotonics

Supervisor:

Pranav Lanka

Co-Supervisor: Rekha Gautam



#### Background:

A Raman spectrum is not only sensitive to the molecular composition, but also to the structure, conformation, and environment of the molecule and therefore has the potential to provide analytical information of interest on a variety of biomolecules. However, the currently used Raman measurement method lacks accuracy and robustness in the quantification of subsurface (deeper) information. The key limitations come from (i) a change in sampling volume across samples due to varying optical properties (absorption coefficient 'µa' and scattering coefficient 'µs') affecting the propagation of both excitation and Raman light and (ii) interfering signals from the top layer.

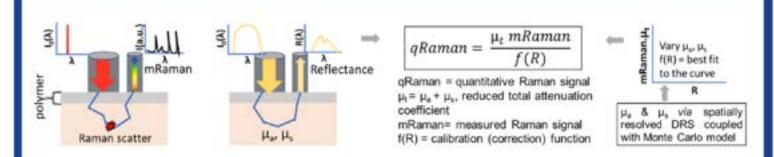
Methods: This project is related to the development of a method to obtain subsurface (deeper) Raman spectra corrected for the optical attenuation (diffuse reflectance) providing accurate concentrations of the biochemicals present in the sample under investigation (such as bone, blood). Raman scattering at a given wavelength ( $\lambda$ ) is proportional to elastically scattered (diffuse reflectance) light at that  $\lambda$  and thus diffuse reflectance spectroscopy (DRS) can aid the corrections in sampling volume.

The intern will be undertaking research activities in Biophotonics group at Tyndall National Institute. Her/his research area will be data acquisition and analysis of Raman and DRS spectra.

Experimental activities: Time-resolved DRS will be incorporated to obtain μa and μs at various depths from the shape of the time-of-flight curve using analytical/numerical model. Raman data will be acquired by varying μa and μs of the samples. Same geometry will be used to acquire DRS spectra to evaluate the correction function.

<u>Theoretical activities:</u> Data analysis will involve some pre-processing including- fitting, background correction, normalization. Further, experimental data coupled with the Photon Migration Theory of light propagation in turbid media will be used to find the relation f(R) between the mRaman and qRaman using reflectance (R). Monte Carlo simulations.

The intern will be given training on the optical instrument and data analysis.



#### For more information or if interested in visiting the lab please contact:

Rekha Gautam, rekha.gautam@tyndall.ie Sanathana Konugolu Venkata Sekar, sanathana.konugolu@tyndall.ie

Location: Tyndall

Type: In-person, Hybrid

Key words: Raman and diffuse reflectance spectroscopy, data analysis, Photon Migration Theory, Monte Carlo simulation

Degree(s) that will suit this project: Physics and Computer science

# Development of an implantable light-guiding hydrogel fibre for multiplexed biosensing

Theme: BioPhotonics Supervisor: Kiang Wei Kho

Co-Supervisor: Christopher Burke



#### Background:

The need to manage increasing number of outpatients in an ageing population calls for innovations in remote patient monitoring technology in order to mitigate symptom exacerbations and the associated costly hospital readmission. This is particularly crucial considering the recent pandemic and the over-stretched healthcare system [1]. Hydrogel – a water-filled matrix of crosslinking polymers – has emerged recently as an attractive implantable platform for long-term biosensing purposes, due to its biocompatibility and excellent anti-fouling properties. Moreover, the simplicity of its fabrication as well as its capacity to be moulded into light carrying optical fibres can bring about many application opportunities. However, most implantable biosensors described in the literature target only one biomarker, which is insufficient for physicians to adequately assess health status in certain cases, especially among older, or chronically critically ill patients [2]. To close this gap, we will explore the fabrication of micro-structured hydrogel optical fibre that carries multiple sensing elements for multi-biomarker detection.

#### Methods:

In this project, we will start by fabricating a hydrogel light guiding fibres based on previous published methods. This will include tuning various fabrication parameters to improve the light-guiding performance of the fibres. This is then followed by incorporation of nanosensors into the so-fabricated fibre. Finally, we will then devise a means to create a thin fibre bundle comprising of multiple biomarker-sensing hydrogel fibres. We will then evaluate the performance of such a fibre bundle.

#### Predicted results and impact:

This study will inform us as to the best design strategy for a hydrogel-based implantable multiplexed biosensing platform. This could potentially lead us to develop the smallest implantable platform capable of tracking temporal concentration changes in multiple biomarkers as a means to increase the sensitivity/accuracy of early diagnosis of symptom exacerbation in outpatients; an endeavour that eludes most of existing detection modalities.

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1.https://doi.org/10.1016/j.heliyon.2022.e12091

2.https://doi.org/10.1016%2Fs0065-2423(08)00405-8

Location: Tyndall Type: In-person

Key words: Nanosensor, remote patient biosensing, hydrogel, biomarkers, implantable

Degree(s) that will suit this project: Bioengineering; physics

# Investigating the possibility of in-vivo detection of pathogenic biofilms on urinary catheter via spectroscopic means

Theme: BioPhotonics Supervisor: Kiang Wei Kho

Co-Supervisor: Shree Khrisnamoorthy, Jerry Green





#### Background:

With the increasing demands for implantable medical devices due to the expansion of aging patient population, there is a need to minimize implant-related infections (IRIs), which have an incidence rate in the million [1], and are one of the leading causes of costly hospital readmission, and healthcare associated mortality (between 5 - 25%), particularly among older patients [1,2]. The ability to detect the onset of IRIs is thus of particular importance. Unfortunately, the inability to differentiate benign Bacterial Biofilms (BB) from pathogenic ones directly due to the lack of reliable extracellularly-secreted biomarkers has challenged pre-IRI detection. Currently, cell culture followed by gene-analysis of biofilm specimen remains the standard procedure to diagnose an IRI [1]. Unfortunately, this necessitates explantation of the implants. To this end, we will explore the possibility of a surface-sensitive spectroscopic technique to detect pathogenic biofilm in-vivo. In this study, we will focus on urinary catheter associated IRI as a use-case example.

#### Methods:

In this project, we will grow biofilms on a suitable substrate. Spectra of the biofilms at different time points are then acquired followed by biomolecular analysis, which will be carried out at the School of Microbiology. Statistical analysis will then be carried out to correlate spectroscopic data with bioanalysis results to evaluate pathogenesis detection.

#### Predicted results and impact:

A positive outcome will have huge implications as it provides a route for in-vivo diagnosis of catheter-associated urinary tract infection (C-UTI), which is the most common nosocomial infection [1]. This not only will greenlight our C-UTI research initiative, but also data from this study will be essential in securing funding.

#### References:

1.https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5110396/

2.https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6245375/

Location: Tyndall Type: In-person

Key words: Remote patient biosensing, urinary tract infections, spectroscopy, implant

Degree(s) that will suit this project: Bioengineering; physics

### **Mechanical Testing to Assess** the Suitability of PEGDM Hydrogels as A Substrate for Osteogenesis Monitoring on **Bone-On-Chip Devices**

Theme:

BioPhotonics

Supervisor:

Imanda Jayawardena

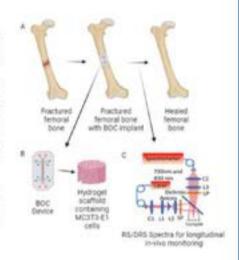
Co-Supervisor: Rekha Gautam





#### Background:

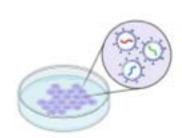
Bone damage affects over 100 million individuals within Europe, totaling €37.5 billion for osteoporotic bone damage alone (Nasello, G., 2021). Traditional treatment approaches involve autologous bone grafting to support osteogenesis, with engineered bone implants becoming a popular regenerative medicine alternative. High failure rates (2-62%) of these implants (Zuo, W., 2016) create a crucial need to improve newly formed bone quality and reduce healing times. A hydrogel-based bone-on-chip (BOC) device coupled to a nonionising optical spectroscopic technique allows for non-invasive, long-term monitoring of osteogenic progression in bone implants, understand bone formation mechanisms on hydrogel scaffolds and evaluate hydrogel scaffold quality.



#### Methods:

Below are research activities that you would be expected to undertake during this project, however, these may vary depending on your preferences as well as the progression of the project. Further information, resources and training would be provided to the successful candidate.

- Prepare PEGDM hydrogels of varying compositions by photopolymerisation with the aid of a photo initiator and a UV light source
- · Acquire Raman spectra of the hydrogel samples
- · Perform mechanical characterisation of cured hydrogel samples
- · Data analysis and interpretation
- Investigating correlations mechanical between properties and pore size of PEGDM hydrogels
- · Optional/Time-Permitting Research Activities
- · Repeat the process for Agarose hydrogels which would be used as a control experiment
- · Cell culture studies on optimal hydrogel substrates





#### Predicted results and impact:

Owing to its ability to promote osteogenesis (Lin-Gibson, S, 2004), the suitability of poly(ethyleneglycol) dimethacrylate (PEGDM) hydrogels as a BOC substrate with respect to its mechanical characteristics would be evaluated in this study. Given adequate time, agarose hydrogels may be evaluated as a control substrate.

#### References:

- [1] Nasello, G., Designing Hydrogel-Based Bone-On-Chips for Personalized Medicine. Appl. Sci. 2021, 11, 4495
- [2] Zuo, W., Investigating clinical failure of bone grafting through a window at the femoral head neck junction surgery for the treatment of osteonecrosis of the femoral head. PLoS One. 2016, 11, e0156903
- [3] Lin-Gibson et al., Synthesis and characterization of PEG dimethacrylates and their hydrogels. Biomacromolecules. 2004, 5, 1280
- [4] Bai, X., Bioactive hydrogels for bone regeneration. Bioact. Mater. 2018, 3, 401
- [5] Joshi, P., Synthesis and characterization of photopolymerizable hydrogels based on poly (ethylene glycol) for biomedical applications. J. Appl. Polym. Sci. 2021, 138, 50489
- [6] Wang, Y., A GelMA-PEGDA-nHA composite hydrogel for bone tissue engineering. Materials. 2020, 13, 3735

#### Contact Information

If you're interested in being part of this cutting-edge Bone-On-a Chip (BOC) Device project, please contact me (Imanda Jayawardena) at imanda.jayawardena@tyndall.ie

Location: Tyndall Type: In-person

Key words: Hydrogels, Medical Devices, Microscopy, Raman Spectroscopy, Cell Culture, Data Analysis Degree(s) that will suit this project: Chemistry, Physics, Biotechnology, Biomedical Engineering

# Fluorescence imaging phantoms for Biophotonics application: fabrication, characterization, validation for surgical guidance and deep tissue application.

Theme: BioPhotonics

Supervisor: Sanathana Konugolu Venkata Sekar Co-Supervisor: Rekha Gautam, Claudia Guadagno





#### Background:

Tissue-mimicking optical phantoms play a crucial role in characterization, optimization, routine calibration and validation of biophotonics systems. The phantoms can be made both in solid or liquid forms, however, solid phantoms have some advantages such as long shelf life, can be molded to realistic organ shapes, stable optical properties (absorption-µa, reduced scattering-µ's), and easy handling for routine instrument validation. In general, a phantom consists of three main components: bulk material (water, epoxy resin, silicone, agar), absorber (India ink, printer toner, black silicone), and scatterer (intralipid, titanium oxide, aluminum oxide, silica microspheres).

This project will develop tissue simulating phantoms to reproduce oxygen saturation seen in human tissue. Intern will participate in the ongoing activity of oxygen saturation phantom developed at FAST-BioPhotonics@Tyndall Lab.

#### Methods:

Wide range of tissue simulation phantoms will be fabricated by making appropriate selection of absorber, scatter, bulk material. The phantoms will be develop to mimic oxygen saturation in range of wavelength (600-1100) relevant to widely available pulse oximeter, oxygen saturation monitors. Predicted results and impact:

Intern will have exposure to both experimental and theoretical work of developing novel phantoms. The activity is align with the labs goal to build next generation phantom tools to standardize the fitness and biomedical parameter monitoring tools in the market, so intern will directly participate in the development of breakthrough technology in this area. In addition, intern will get acedamia/industry collaboration exposure through the industry partner (BioPixS).

#### References:

Sanathana Konugolu Venkata Sekar, Andrea Pacheco, Pierluigi Martella, Haiyang Li, Pranav Lanka, Antonio Pifferi, and Stefan Andersson-Engels, "Solid phantom recipe for diffuse optics in biophotonics applications: a step towards anatomically correct 3D tissue phantoms," Biomed. Opt. Express 10, 2090-2100 (2019)

For more information or if you want to visit our lab please contact: Sanathana Konugolu Venkata Sekar, <u>sanathana.konugolu@tyndall.ie</u>

Location: Tyndall Type: In-person

Key words: Phantoms, standardization, fabrication, polymer/material chemistry, biophotonics

Degree(s) that will suit this project: physics and biomedical engineering

## Tissue simulating blood oxygen saturation phantoms for biophotonics application

Theme:

BioPhotonics

Supervisor:

Sanathana Konugolu Venkata Sekar

Co-Supervisor: Rekha Gautam, Claudia Guadagno





#### Background:

Tissue-mimicking optical phantoms play a crucial role in characterization, optimization, routine calibration and validation of biophotonics systems. The phantoms can be made both in solid or liquid forms, however, solid phantoms have some advantages such as long shelf life, can be molded to realistic organ shapes, stable optical properties (absorption-µa, reduced scattering-µ's), and easy handling for routine instrument validation. In general, a phantom consists of three main components: bulk material (water, epoxy resin, silicone, agar), absorber (India ink, printer toner, black silicone), and scatterer (intralipid, titanium oxide, aluminum oxide, silica microspheres).

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#### Methods:

Wide range of tissue simulation phantoms will be fabricated by making appropriate selection of absorber, scatter, bulk material. The phantoms will be develop to mimic oxygen saturation in range of wavelength (600-1100) relevant to widely available pulse oximeter, oxygen saturation monitors. Predicted results and impact:

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#### References:

Sanathana Konugolu Venkata Sekar, Andrea Pacheco, Pierluigi Martella, Haiyang Li, Pranav Lanka, Antonio Pifferi, and Stefan Andersson-Engels, "Solid phantom recipe for diffuse optics in biophotonics applications: a step towards anatomically correct 3D tissue phantoms," Biomed. Opt. Express 10, 2090-2100 (2019)

For more information or if you wanna visit our lab please contact: Sanathana Konugolu Venkata Sekar, sanathana.konugolu@tyndall.ie

Location: Tyndall Type: In-person

Key words: Phantoms, standardization, fabrication, polymer/material chemistry, biophotonics

Degree(s) that will suit this project: physics and biomedical engineering

### CMOS amplifier design for sensor interfaces

SOLVE THE IMPOSSIBLE

Theme: Circuit Design Supervisor: Daniel O'Hare

Co-Supervisor: Rekha Gautam, Claudia Guadagno

#### Background:

We live in an Internet of Things (IoT) world where our environment and vital signs are monitored by hundreds of different sensors. Each iteration of the leading Smartphones incorporate more and more sensors. A traditional multisensor Analogue Frontend (AFE) consists of separate channels from each sensors. Each signal path has custom Amplifiers and Filters and there is a shared Analogue to Digital Converter (ADC) to digitise the signals. In this project we want to use our Python based design tool pygmid to design Amplifier and Filters for sensor interface circuits.



#### Methods:

The intern will learn to design amplifier circuits using our Python based design tool. There will be opportunities to test the designed amplifiers using Cadence simulation tools. There will also be opportunities to do some lab based measurements of sensor interface circuits previously designed in our group.

#### Predicted results and impact:

The intern will get an opportunity to experience the complete design and test cycle of an integrated circuit. They will learn how to use our Python based tool pygmid and industry standard tools such as Cadence and they will learn about the applications where some of our sensor interface circuits are used.

#### References:

Razavi, Behzad. Fundamentals of microelectronics. John Wiley & Sons, 2021.

Jespers, P., & Murmann, B. (2017). Systematic Design of Analog CMOS Circuits: Using Pre-Computed Lookup Tables. Cambridge: Cambridge University Press. doi:10.1017/9781108125840

Location: Tyndall Type: In-person

Key words: Integrated Circuit (IC) design, analogue circuits, CMOS, amplifiers, sensor interfaces

Degree(s) that will suit this project: Electrical/Electronic Engineering

### Electric Field Control of Skyrmionic Spin Patterns in 2D Multiferroelectric Materials

Theme: Emerging Materials & Devices / Materials Theory

Supervisor: Mohammad Noor-A-Alam

Co-Supervisor: Michael Nolan



#### Background:

Skyrmions are topologically stable, vortex-like spin textures that have garnered significant attention in the field of condensed matter physics. These structures are characterized by swirling spin arrangements that can exist in certain magnetic materials. While Skyrmions are primarily associated with magnetic systems, there is growing interest in exploring their presence in multiferroic materials. Multiferroelectric materials exhibit both ferroelectric and magnetic properties. In recent research, the potential for coupling between the electric and magnetic order in multiferroelectrics has been explored to control Skyrmions. The interplay between these two types of order parameters in multiferroelectrics offers a unique platform for the creation and manipulation of Skyrmions.

The presence of Skyrmions in multiferroic materials has sparked excitement due to the potential for novel technological applications. For example, the ability to control Skyrmions using an external electric field offers the promise of low-power, electrically tuneable devices for data storage and processing. Additionally, the study of Skyrmions in multiferroelectric materials contributes to a deeper understanding of the complex interplay between different order parameters in complex materials.

This research project focuses on the investigation of 2D multiferroelectric materials, specifically examining VOl2 and similar monolayer structures. Our primary objective is to manipulate the chirality of Skyrmions by switching the ferroelectric polarization using an electric field. This alteration in polarization, in turn, modulates the chirality of Dzyaloshinskii-Moriya interactions (DMIs) that play a pivotal role in the formation and characteristics of Skyrmions.

#### Methods:

The Monte Carlo method, when coupled with Density Functional Theory (DFT), provides a versatile and powerful framework for investigating the intricate properties and behaviours of Skyrmions in magnetic materials. DFT offers a fundamental basis for understanding the electronic and magnetic structures of materials, providing critical input parameters such as exchange interactions and anisotropy energies. Monte Carlo simulations then take these parameters and explore the complex dynamics of Skyrmions within the material. By randomly sampling different spin configurations and using Metropolis-based algorithms to determine their energy states, we will gain insights into the thermodynamics and stability of Skyrmions, their response to external fields, and the construction of phase diagrams for various magnetic orders. This integrated approach bridges the theoretical foundation of DFT with the statistical and dynamic exploration of Monte Carlo simulations, facilitating a comprehensive understanding of Skyrmions and their potential applications in the realm of advanced materials and technology.

#### Predicted results and impact:

- To predict the conditions under which Skyrmions are likely to form within a magnetic material. By varying parameters such as temperature, magnetic field strength, and exchange interactions, we will identify the range of conditions that favour Skyrmion formation.
- To estimate their thermodynamic properties, including the energy, entropy, and specific heat associated with Skyrmions. This information is crucial for understanding the stability and behaviour of Skyrmions as a function of temperature.
- To predict the mobility of Skyrmions in response to external fields. By predicting how easily Skyrmions can be manipulated and moved, we can assess their utility in applications like data storage and magnetic logic devices.
- To predict how Skyrmions respond to external magnetic field or change in temperature. These
  predictions aid in designing and optimizing Skyrmion-based devices and systems.

#### References:

- 1. Large piezoelectric response in ferroelectric/multiferroelectric metal oxyhalide MOX2 (M = Ti, V and X = F, Cl and Br) monolayers, Mohammad Noor-A-Alam and Michael Nolan, Nanoscale 2022, 14, 11676 https://doi.org/10.1039/D2NR02761E
- 2. Negative Piezoelectric Coefficient in Ferromagnetic 1H-LaBr2 Monolayer, Mohammad Noor-A-Alam, and Michael Nolan, ACS Applied Electronic Materials 2022, 4, 2, 850-855 DOI: 10.1021/acsaelm.1c01214
- 3.Electric-Field Switching of Magnetic Topological Charge in Type-I Multiferroics, Changsong Xu, Peng Chen, Hengxin Tan, Yurong Yang, Hongjun Xiang, and L. Bellaiche, Physical Review Letters 2020, 125, 037203 DOI: 10.1103/PhysRevLett.125.037203

Location: Tyndall Type: In-person

Key words: Monte Carlo method, Skyrmions, multiferroic materials, 2D materials, simulation, electric field, magnetic field, monolayer

Degree(s) that will suit this project: Physics, Mathematical/Theoretical Physics, Materials Science, Chemical Physics and Mathematics

### Machine Learning Approaches for Enhanced Magnetic Response in Novel Multiferroic Devices

Emerging Materials & Devices / Materials Theory

Supervisor: Michael Nolan Co-Supervisor: Florentino Silva



#### Background:

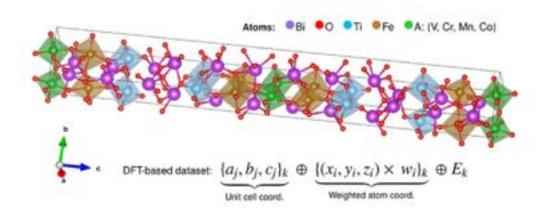
Theme:

Multiferroic (MF) materials are single phase materials that exhibit simultaneous ferroelectric and ferromagnetic responses. This rare class of material could be used to develop a new type of data-storage which stores 4 to 8 bits in a single cell tunnel junction - whilst current memory architectures work on 2 bits tunnel junctions. Once well understood, this material will pave the way for next-generation memory devices that deliver higher storage densities, way beyond current technology. However, stable, room temperature operating multiferroics are very rare as ferroelectric and ferromagnetic properties tend to be exclusive.

As a candidate multiferroic material, our research focus on the characterization of Aurivillius phase Bi(m+1) TixFeyMnzO3(m+1), considering five blocks (so-called m=5) of perovskites sandwiched by Bismuth oxide (Bi2O2)2+ layers. From the computational modelling perspective, this material imposes some challenges. Firstly, the large unit cell comprises 116 atoms. Secondly, the Bismuth oxide layer is an interface that is fundamental for the structure stability. Lastly, its composition relies on 5 different atomic species, each of them with distinct electronic properties and oxidation states.

#### Methods:

Our computational approach uses Density Functional Theory (DFT) to characterize the most stable arrangements of metal species in Aurivillius multiferroics. To overcome the computational cost and size limitations imposed by DFT calculations, we have started implementing machine learning (ML) models that are trained on DFT results with unit cells that have a size of the order of 100 atoms, which with ML is easily expandable to 1000 atoms to study more realistic structures, exploiting the ML models to make these calculations feasible for the first time.



#### Predicted results and impact:

In this project, we will explore different compositions of our novel multiferroics by replacing the magnetic cation A (which can be one of V, Cr, Mn, Co) in the central layer of the perovskite block. This project will be divided in three parts. In the first part, the student will learn how to use the software and techniques required, namely DFT concepts, molecule visualisation, and Python ML packages. The student will be introduced to recent results on the DFT and ML interface developed by our group. In the second part, the student will work on ML simulations based on the DFT results for each of the magnetic cation A of interest. This step will involve data engineering and model benchmarking. Finally, the student will explore super-cell properties by comparing DFT and ML results. It is expected that the project will explore a broad ecosystem of ML methods, namely statistical learning, neural networks and gaussian approximation potential, to assess the most suitable approach for ML driven discovery of novel complex multiferroic materials.

#### References:

- [1] Wang, Anthony Yu-Tung, et al. "Machine learning for materials scientists: an introductory guide toward best practices." Chemistry of Materials 32.12 (2020): 4954-4965.
- [2] Florentino Silva, Michael Sweetman and Michael Nolan. 'Machine Learning Modelling of Multiferroic Bi5Ti3FeO15 SupercellStructures'. In: Chemistry Final Year Project, University College Cork (January 2023).
- [3] Florentino Silva, Orla Fitzmaurice and Michael Nolan. 'Machine Learning Approach for Predicting Stable Distributions onMultiferroic Bi6Ti3Fe2O18'. In: Summer Fellowship Programme, Tyndall National Institute (August 2022).

Location: Tyndall Type: In-person

Key words: Multiferroics, machine learning, DFT, oxides, magnetism

**Degree(s) that will suit this project:** The project is suited to students with a Physics, Chemistry or Mathematics background. The important topics to be emphasized will be tailored depending on the student background.

# Laser induced graphene based electrochemical sensing devices for sweat analysis.



Tyndall

Theme:

Emerging Materials & Devices / Nanotechnology

Supervisor: Hassan Hamidi

#### Background:

Electrochemical (bio)sensors leverage oxidation-reduction reactions, measuring corresponding electron transfer through changes in current, voltage, or other parameters using diverse electrochemical techniques. The utilization of electrochemically active materials plays a crucial role in ensuring the efficacy of these (bio)sensors. Laser-induced graphene (LIG) has become increasingly prominent in the realm of biosensor development and enhancement due to its notable attributes such as high electrical conductivity, specific surface area, and a straightforward and scalable fabrication process1-4. The primary focus of this project will be the construction and the evaluation of analytical characteristics of the sensing platforms.

#### Methods:

The intern will acquire experimental skills in constructing electrochemical biosensors. This involves learning the direct laser writing (DLW) technique to fabricate electrode features on substrates such as polyimide and bioplastics. They will then employ various functionalization strategies to build (bio)sensors capable of detecting important biomarkers and electrolytes in sweat. The primary focus of the project will be evaluating the analytical characteristics and performance of the developed biosensors.

#### Predicted results and impact:

Predicted results:

- High performance biosensing devices for non-invasive sweat analysis developed and tested.
- · Stretch Goal:
- Utilisation of the developed biosensors for real-time and multiplexed monitoring of the biomarkers level in sweat.

#### Impact:

- · The developed sensing platform has a great potential for a reliable diagnostic device.
- Research paper
- · Conference presentation

#### References:

- Vivaldi, F. M.; Dallinger, A.; Bonini, A.; Poma, N.; Sembranti, L.; Biagini, D.; Salvo, P.; Greco, F.; Di Francesco, F. ACS Appl. Mater. Interfaces 2021, 13 (26), 30245–30260. https://doi.org/10.1021/acsami.1c05614.
- 2. Madden, J.; Vaughan, E.; Thompson, M.; O' Riordan, A.; Galvin, P.; Iacopino, D.; Rodrigues Teixeira, S. Electrochemical Sensor for Enzymatic Lactate Detection Based on Laser-Scribed Graphitic Carbon Modified with Platinum, Chitosan and Lactate Oxidase. Talanta2022, 246, 123492. https://doi.org/https://doi.org/10.1016/j.talanta.2022.123492.
- Vaughan, E.; Santillo, C.; Setti, M.; Larrigy, C.; Quinn, A. J.; Gentile, G.; Lavorgna, M.; Iacopino, D. Adv. Sens. Res. 2023, n/a (n/a), 2300026. https://doi.org/https://doi.org/10.1002/adsr.202300026.
- 4. Hamidi, H.; Levieux, J.; Larrigy, C.; Russo, A.; Vaughan, E.; Murray, R.; Quinn, A. J.; Iacopino, D. Biosens. Bioelectron. X 2023, 15, 100403. https://doi.org/https://doi.org/10.1016/j.biosx.2023.100403.

Location: Tyndall Type: In-person

Key words: Biosensors, ion sensing, electrochemistry, sweat analysis, laser induced graphene.

Degree(s) that will suit this project: Analytical chemistry.

# Development of cortisol textile sensors

Tyndall

Theme:

Emerging Materials & Devices / Nanotechnology

Supervisor: Daniela Iacopino

#### Background:

Flexible wearable sweat sensors allow continuous, real-time, non-invasive detection of sweat analytes, provide insight into human physiology at the molecular level, and have received significant attention for their promising applications in personalized health monitoring. Electrochemical sensors are the best choice for wearable sweat sensors due to their high performance, low cost, miniaturization, and wide applicability. While most electrochemical sensors are fabricated on rigid substrates, there is a growing need for sensors that can be manufactured on inexpensive and flexible materials. In the last five years the NTG group has developed expertise in direct laser writing of graphene-like electrode materials. Such electrodes have been used for electrochemical sensing and biosensing [1-3], energy storage and harvesting [4]. In this project we want to develop strategies for the fabrication of textile cortisol sensors by using direct laser writing techniques on Kevlar textiles or conductive threads.

Here, we present a unique embroidered electrochemical sensor that is capable of quantitative analytical measurements using raw biofluid samples. Conductive threads immobilized with enzyme probes were generated using a simple and robust fabrication process and used to fabricate flexible, mechanically robust electrodes on textiles. For proof of concept, measurements were performed to detect glucose and lactate in buffer and whole blood samples, which exhibited excellent specificity and accuracy. We also demonstrate that our embroidered biosensor can be readily fabricated in two-dimensional (2D) arrays for multiplexed measurements. Lastly, we show that this biosensor exhibits good resiliency against mechanical stress and superior repeatability, which are important requirements for flexible sensor platforms

#### Methods:

Fabrication of conductive threads from graphene-like inks or by direct laser writing of kevlar

#### Predicted results and impact:

Demonstration of biosensing (cortisol) in buffer and artificial sweat on embroidered sensor platforms

#### References:

- [1] Hamidi, H. et al Biosensors and Bioelectronics: X 15, 100403, 2023
- [2] Vaughan, E. et al ACS Sustainable Chemistry & Engineering 11 (37), 13574-13583, 2023
- [3] Vaughan, E. et al Advanced Sensor Research, 2300026
- [4] Imbrogno, A. et al ACS Applied Electronic Materials 4 (4), 1541-1551

Location: Tyndall Type: In-person

Key words: smart textiles, direct laser writing, cortisol biosensor

Degree(s) that will suit this project: Chemistry, analytical chemistry, nanotechnology

### Hierarchical heteronanostructure catalyst for biosensors

Tundall

Theme: Emerging Materials & Devices / Nanotechnology Supervisor: Padmanathan Narayanasamy



#### Background:

Digital biosensor technologies are advancing healthcare applications by providing integrated applications to monitor personalized fitness and health problems on a daily basis. For sanitary reasons, sustainable health-monitoring sensors such as glucose, pH, temperature, stress/strain, and other target biosensors are desirable [1]. Electrochemical biosensors are appealing among the several reported sensors for ultra-trace detection biomolecules in the food sector and healthcare applications. Unique approaches and nanostructures have been used in the upsurge of nanotechnology research to bring unique expansion to current biosensors [2]. Hierarchically heterostructured materials with synergistic surface accessibility, large surface area, and interrelated hierarchical porosity at varied lengths shown outstanding electrochemical activity for biosensors, gas detection, and energy storage. In fact, cost-effective and biocompatible catalysts are critical in the development of biosensors for food and health care applications [3]. This project will evaluate selective detection of target biomolecules and pH sensing using hierarchical hetero-metal oxide nanostructures and their synergistic contribution, which will be validated further to increase selectivity and sensitivity towards different analytes.

#### Aim and Objective of Project

- The aim of this project is to design hierarchical hetero-nanostructure-based biosensors for the selective detection of any of the target analytes (e.g., glucose, lactose, dopamine, cortisol, etc.).
- The sensitivity and selectivity of the developed sensors will be investigated in commercial food
  products to validate the catalyst for practical device fabrication.
- By virtue of its multifunctionality, a synthesized hierarchical hetero-structure can be investigated for pH sensing in commercial beverages.

#### Methods:

Design and the fabrication of hierarchical hetero-metal oxide nanostructured catalyst via electrodeposition or wet chemical methods.

Analytical characterization of the catalyst applying X-Ray diffraction, scanning electron microscopy and Raman spectroscopy.

Electrochemical biosensor fabrication and testing using cyclic voltammetry and chronoampermetry techniques.

#### Predicted results and impact:

This project's biosensor will benefit researchers in developing ultra-trace detection of biomolecules for early diagnosis and food quality analysis. If this study is successful, the proposed device could have a significant impact on digital technologies integrated biosensors for continuous health care applications. The fellow researcher will gain an understanding of what constitutes a biosensor and how it is designed and utilized for various technological application.

#### References:

- [1] Gao, Wei, et al. "Fully integrated wearable sensor arrays for multiplexed in situ perspiration analysis." Nature 529 (7587), 2016: 509-514.
- [2] Lee, Hyunjae, et al. "A graphene-based electrochemical device with thermoresponsive microneedles for diabetes monitoring and therapy." Nature nanotechnology 11.6 (2016): 566-572.
- [3] Hassan, Israr U., et al. "A review on recent advances in hierarchically porous metal and metal oxide nanostructures as electrode materials for supercapacitors and non-enzymatic glucose sensors." Journal of Saudi Chemical Society 25(5), 2021:101228.

Location: Tyndall Type: In-person

Key words: Biosensor, catalyst, analytes, sensitivity and food analysis

Degree(s) that will suit this project: Chemistry, Physics, Engineering Science, Material Science

# Detection of PFAS (per- and poly-fluoroalkylated substances) in river water

Theme: Emerging Materials & Devices

Advance nano sensor

Supervisor: Tarun Narayan Co-Supervisor: Alan O'Riordan



#### Background:

PFAS very large group of man-made chemicals that have multiple fluorine atoms attached to a carbon chain. They can have harmful effects on human and animal health and stay in the environment and in our bodies for long periods of time where they can increase in concentration. They are often referred to as "forever chemicals". Some PFAS have been linked to an increased risk of cancer, high cholesterol, reproductive disorders, hormonal disruption (also known as endocrine disruption) and weakening of the immune system. The aim of the project will be detecting these compounds using electrochemical sensors. This would help to tackle the problem of PFAS in environment. These sensors could replace the current detection techniques, which will help in purifying the water samples.

#### Methods:

The project will involve working with smart materials that can selectively detect the PFAS in the environment. The next part would be integrating these sensors in our fabricated electrodes for detection of PFAS.

#### Predicted results and impact:

These sensors will be deployed near river water for the detection of PFAS. Within the project, the sensor will be developed to provide real-time PFAS level data.

#### References:

A Practical Beginner's Guide to Cyclic Voltammetry | Journal of Chemical Education (acs.org), Voltammetric Determination of Phosphate in Brazilian Biodiesel Using Two Different Electrodes -Torrezani - 2011 - Electroanalysis - Wiley Online Library.

Location: Tyndall Type: In-person

Key words: electrochemical; sensors; environmental monitoring; PFAS; Carbon based materials.

Degree(s) that will suit this project: Chemistry and Bio-chemistry

# Analysis of energy efficiency measures applicable in energy intensive industries

IERC

Theme: Energy

Supervisor: Luciano De Tommasi

#### Background:

The IERC is the coordinator of the EU project Audit Plus (Enhancing energy audit schemes in Energy Intensive Industries with practical approaches), funded under European LIFE-CET-22 call [1]. Audit Plus started its activities in October 2023. The project will enhance energy audit schemes in Energy Intensive Industries (EII) with practical approaches, providing technical, financial, regulatory and training support to these industries. EII are those manufacturing industries that use high amounts of energy, and for which the proportion of energy costs compared to production costs is high. Audit Plus will act as a one-stop shop that will offer an integral energy efficiency consultancy service to 82 energy intensive industries of the pharmaceutical, chemical and healthcare sectors in Ireland, ceramic sector in Castellon (Spain), fishing and food processing sectors in Galicia (Spain), food processing sector in Poland. The integral service offered by Audit Plus will include the following features:

- 1.technology assessment
- 2.cost-benefit analysis
- 3. engineering support
- 4. identification of public and private sources for financing
- 5. matchmaking between energy intensive industries and technology/service providers
- 6.guidance for implementing recommended energy efficiency measures after energy audits plans
- 7. consultancy to develop a corporate energy strategy

Moreover, Audit Plus will develop a knowledge hub for energy efficiency in energy intensive industries that will be made publicly accessible via the World Wide Web.

Methods: The intern will contribute to the review of energy efficiency measures applicable to EII already started by IERC and to the development of a case study. These activities will contribute to the technology assessment service offered by IERC to a number of EII of the pharmaceutical, chemical and healthcare sectors in Ireland as well as to EII of other sectors as part of the Audit Plus integral service [2-4]. The Fellow will contribute to the development of a case study for a specific EII using available information about:

- 1.technical description of energy efficiency measures
- potential energy savings and energy cost reductions delivered by each measure
- 3. installation costs
- 4. boundaries for measures' applicability.

**Predicted results and impact:** The project will contribute to the implementation of the technology assessment service for the assessment of energy efficiency measures in EII led by IERC in the Audit Plus project. It is expected that the Fellow will deliver a short report recommending a set of energy efficiency measures for a specific industry.

#### References:

- [1] https://www.ierc.ie/improving-energy-efficiency-in-energy-intensive-industries-call-forstakeholders-interested-in-the-irish-market/
- [2] Li, M. J., & Tao, W. Q. (2017). Review of methodologies and polices for evaluation of energy efficiency in high energy-consuming industry. Applied Energy, 187, 203-215.
- [3] Bruni, G., Martini, C., Martini, F., & Salvio, M. (2023). On the Energy Performance and Energy Saving Potential of the Pharmaceutical Industry: A Study Based on the Italian Energy Audits. Processes, 11(4), 1114.
- [4] Hohne, P. A., Kusakana, K., & Numbi, B. P. (2020). Improving energy efficiency of thermal processes in healthcare institutions: A review on the latest sustainable energy management strategies. Energies, 13(3), 569.

Location: Tyndall Type: Hybrid

Key words: energy efficiency measures, energy intensive industries

Degree(s) that will suit this project: Energy Engineering, Electrical Engineering, Mechanical Engineering and similar.

### Fabrication and optimization of an electrochemical sensor for monitoring the welfare of fish

Theme: Integrated Sensors / Life Science Interface

Supervisor: Sofia Rodrigues Teixeira



Tyndall
National Institute

#### Background:

Animal health and welfare are issues of high research priority for the European aquaculture industry. In particular, improving animal welfare whilst reducing the use of veterinary drugs are current research priorities in line with minimising the environmental impact of the industry [1,2], and ensuring that consumers can trust that their food is produced to the highest international standards. As part of an overall programme to develop a multiparameter sensing system for monitoring wellbeing of fish in aquaculture facilities, this project will involve fabrication and optimisation of a flexible electrochemical immunosensors, as a biomarker for monitoring the welfare of selected fish species.

#### Methods:

The evaluation of the sensor will involve testing various attachment chemistries and optimizing the sensor's performance in buffer solutions for a designated target.

Predicted results and impact: The sensor to be developed will be integrated as part of a multiparameter sensor solution to enable minimally invasive real-time monitoring of the fish at the production facility.

#### References:

[1] Carballeira Braña CB, Cerbule K, Senff P and Stolz IK (2021) Towards Environmental Sustainability in Marine Finfish Aquaculture. Front. Mar. Sci. 8:666662. doi: 10.3389/fmars.2021.666662

[2] Ahmed, N., Thompson, S. & Turchini, G.M. Organic aquaculture productivity, environmental sustainability, and food security: insights from organic agriculture. Food Sec. 12, 1253-1267 (2020). https://doi.org/10.1007/s12571-020-01090-3

Location: Tyndall Type: In-person

Key words: Electrochemical sensor; Printing; Flexible; Welfare; Animal.

Degree(s) that will suit this project: engineering, Materials Engineering, Biomedical engineering.

## Fabrication of on-chip Electrochemiluminescence (ECL) Aptamer sensing platform for pint-of-care (POC) application

Theme: Integrated Sensors / Nanotechnology

Supervisor: Somayyeh Bozorgzadeh



#### Background:

The development of compact biosensing devices capable of sensitive and selective concomitant detection of two or more analytes in a single sample has enormous potential for point-of-care and use applications. Silicon microfabrication technologies outperforms other fabrication processes in reproducibility, miniaturization capability, and design adjustability Electrochemiluminescence (ECL) refers to the light emission induced by the redox reaction occurring on the electrode surface. Nowadays, (ECL) has become an important and promising method for biosensors due to the advantages of low background, being easily control and high sensitivity uncomplicated operation, wide response range and cost-effective instruments. On the other hand, Aptamers are artificial oligonucleotides (DNA or RNA) selected in vitro that recognize a broad scope of analytes with good affinity and specificity. Recently, biosensors that combine the excellent sensitivity of the ECL and good specificity of aptamers have been developed rapidly. Hence, this project aims to leverage on-silicon chip multiplexed sensing array platforms for construction an ECL biosensor with an aptamer recognition layer, 3-5

#### Methods:

In this summer project, the intern will gain experience in the fabrication of aptamer biosensor. This includes tasks such as electrode modification, aptamer immobilisation, electrochemical and ECL characterisations and measurements. Finally, the analytical application of the designed biosensor will be evaluated.

#### Predicted results and impact:

Predicted results:

· On-chip ECL aptamer biosensing platform developed and tested.

#### Stretch Goal:

· Adaption the designed ECL aptamer biosensing platform for multiplexed analysis

#### impact

- ECL aptamer sensor has a great potential for sensitive point-of-care applications.
- · Research paper
- · Conference presentation

#### References:

- 1. Juska, V. B., Maxwell, G. D. & O'Riordan, A. Microfabrication of a multiplexed device for controlled deposition of miniaturised copper-structures for glucose electro-oxidation in biological and chemical matrices. Biosens. Bioelectron. X 13, 100315 (2023).
- Juska, V. B., Maxwell, G., Estrela, P., Pemble, M. E. & O'Riordan, A. Silicon microfabrication technologies for biology integrated advance devices and interfaces. Biosens. Bioelectron.237, 115503 (2023).
- Padmakumari Kurup, C., Abdullah Lim, S. & Ahmed, M. U. Nanomaterials as signal amplification elements in aptamer-based electrochemiluminescent biosensors. Bioelectrochemistry 147, 108170 (2022).
- 4. Yang, X. et al. Electrogenerated chemiluminescence biosensor array for the detection of multiple AMI biomarkers. Sensors Actuators B Chem. 257, 60–67 (2018).
- Cánovas, R. et al. Novel electrochemiluminescent assay for the aptamer-based detection of testosterone. Talanta239, 123121 (2022).

Location: Tyndall Type: In-person

**Key words:** Electrochemiluminescence, aptamer sensor, On-silicon chip sensing array platform, Multiplexed analysis.

Degree(s) that will suit this project: Chemistry and Biochemistry

# Modelling of InGaN based nanostructures for energy-efficient green gap range light emitters.

Theme:

Monolithic & Heterogeneous Integrations

Photonics Theory

Supervisor:

Amit Kumar Singh

Co-Supervisor: Stefan Schulz



#### Background:

III-Nitride semiconductors (AIN, InN, GaN and their alloys) have attracted significant research interest given their importance for displays, solid-state lighting, visible-light communication and biomedical applications. Indium gallium nitride (InGaN) alloys offers tremendous potential for developing compact, reliable, environment friendly, low-power and wavelength-tunable light-emitters since its wide band gap covers the wavelength window from near UV up to near-infrared range by tailoring the alloy content. InGaN light-emitting diodes (LEDs) have achieved maximum external quantum efficiency (EQE) over 80% in the violet-blue spectral range. However, expansion to green and further to yellow spectral range leads to much lower maximum EQEs, also known as the green gap problem [1]. To theoretically guide the design of these light emitters accurate modelling of InGaN alloys is required. Detailed information on how the electronic band parameters change with alloy composition are a crucial ingredient for an accurate modelling. This information is, however, often not available, and parameters are generally obtained by linear interpolation between the binary material components; given the strong carrier localization effects in InGaN alloys [2], such an approach is most likely not a good approximation, which consequently leads to uncertainties in device simulations.

#### Methods:

First principles calculations such as the density functional theory (DFT) allow the prediction of material properties on the foundations of quantum mechanics. We will start by utilizing DFT to derive effective electronic band structures of the ternary alloys (InxGa1-xN). Small supercells present in general a problem when predicting properties of systems which exhibit carrier localization effects. This stems from the fact that small supercells result in long-range ordering effects which may mask the local alloy effects. Taking this into account, large InGaN supercell structures with random distributions of In and Ga atoms will be considered. While atomistic DFT simulations are highly accurate, they are computationally too expensive to simulate a full device. Thus, simpler continuum-based models such as the so-called k-p method remain the workhorse for most device simulations. k-p method is a perturbation-based approach of calculating energy bands and wavefunctions in the vicinity of band edges. By fitting continuum-based k-p band structures to the DFT results, using the k-p parameters as free and adjustable parameters, will allow to transfer the local alloy effects in the k-p method. The k-p parameter sets extracted through this approach shall provide the basis for designing InGaN based energy-efficient green gap light emitters.

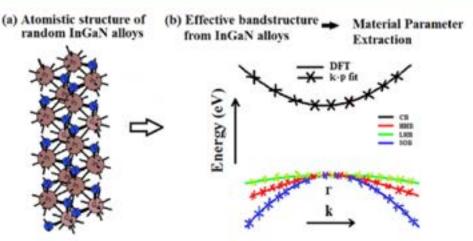


Fig. 1. Steps in k-p parameter extraction for InGaN alloys (a) generation of random InGaN alloys (b) Calculation of effective bandstructure using first principles approach and fitting of first principles bandstructure with k-p method. CB, HHB, LHB and SOB stand for conduction band, heavy hole band, light hole band and split-off band respectively.

#### Predicted results and impact:

- Training on calculating electronic band structures of materials from atomistic DFT on high performance clusters.
- · Experience of working on a multiscale simulation framework.
- · Possible contribution to research article.

#### References:

[1] Karpov, Sergey Yu., Carrier localization in InGaN by composition fluctuations: implication to the "green gap", Photonics Research 5, 2017

[2] Jeong, Hyun et al., Redistribution of carrier localization in InGaN-based light-emitting diodes for alleviating efficiency droop, Journal of Luminescence, 252, 2022

Location: Tyndall Type: Hybrid

Key words: Modelling, DFT, nanostructures, semiconductors, photonics

Degree(s) that will suit this project: Engineering (Computer, Electronics), Physics, Mathematics

# Predicting fundamental properties of boron containing nitride semiconductors from atomistic models for use in future energy efficient light emitters.



Theme: Monolithic & Heterogeneous Integrations

Photonics Theory

Supervisor: Cara-Lena Nies

Co-Supervisor: Stefan Schulz



#### Background:

The group III-Nitride (III-N) semiconductors (AIN, GaN, InN) and their alloys ((Al,Ga,In)N) have attracted significant interest in manufacturing energy efficient optoelectronic devices such as light emitting diodes (LEDs). In principle, by adjusting the alloy composition in Al1-x-yGaxInyN, the emission wavelength of devices utilizing these materials can be tuned to spectral regions ranging from deep ultraviolet (UV) to red. However, both UV LEDs made from (Al,Ga)N and red LEDs made from (In,Ga)N, suffer from poor efficiencies. One property that impacts the overall properties of III-N materials is their material specific, built-in polarisation, also referred to as spontaneous polarisation. Additionally, so-called piezoelectric polarisation can arise due to strain in the active region of a device. Strain might be caused by size mismatch when growing layers of different materials or arise from size differences between the components of the alloy, e.g. In atoms are larger than Ga atoms. Recently, the addition of boron to III-N alloys has emerged as an option to combat the efficiency challenge. Despite significant interest in these novel alloys, many of the fundamental properties, including polarisation effects, of boron containing III-N alloys are not yet well studied and consequently understood. Polarisation properties are especially important when designing heterostructures, such as quantum well systems, for optoelectronic devices using these materials, as any discontinuity in electric polarisation fields results in the formation of sheet charges at interfaces and thus electrostatic built-in fields [1]. In particular, we are interested in understanding the effect of the alloy microstructure on the polarisation and overall electronic properties, as microstructure can significantly alter e.g., the band gap[2]. Understanding these properties, for ternary (B)-III-N alloys, but especially for the quaternary alloys (B,Al,Ga)N and (B,In,Ga)N is not trivial, but will significantly support both theoretical and experimental design of devices made from boron containing nitrides.

#### Methods:

The properties of boron containing nitrides will be computed from state-of-the art first-principles atomistic simulations. In particular, we will use density functional theory (DFT) to model B-III-N alloys. From these calculations, we aim to extract the relevant parameters to help us understand the polarisation properties using the method detailed by Dreyer et al.[2]

#### Predicted results and impact:

The scientific aim of this summer project is to advance understanding of the fundamental properties of B-III-N alloys, with a particular focus on polarisation fields. Understanding of these properties is currently lacking in the literature and thus any results are likely to lead to a publication in the future. The student working on this project will learn to (i) perform state-of-the-art DFT calculations, (ii) create models of complex alloys and (iii) gain an understanding of the underlying mechanisms that create built-in polarisation fields in realistic nitride materials.

#### References:

[1] Dreyer, C. E., Janotti, A., Van de Walle, C. G., & Vanderbilt, D. (2016). Physical Review X, 6(2). DOI: 10.1103/PhysRevX.6.021038

[2] Nies, C. L., Sheerin, T. P., & Schulz, S. (2023). APL Materials, 11(9). DOI: 10.1063/5.0171932

Location: Tyndall Type: Hybrid

Key words: computational physics, atomistic simulations, nitride materials, optoelectronic devices, piezoelectricity, polarisation

Degree(s) that will suit this project: Physics, Chemical Physics

# Theory of hexagonal gallium phosphide as a green-wavelength light emitter

Theme: Monolithic & Heterogeneous Integrations

Supervisor: Christopher Broderick

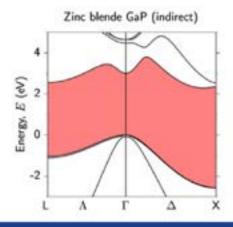


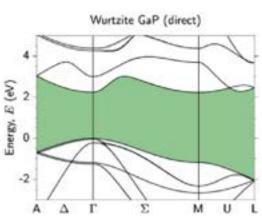
#### Background:

III-V semiconductors, which are ubiquitous in practical applications ranging from optical communications and sensing to microelectronics and photovoltaics, crystallise in one of two crystal structures. III-N compounds crystallise in the hexagonal wurtzite structure, while III-(P,As,Sb) compounds crystallise in the cubic zinc blende structure. Advances in semiconductor nanowire fabrication allow to fabricate III-(P,As,Sb) compounds in the wurtzite structure.

The efficiency of light emission from a semiconductor is determined by its electronic band structure – i.e. the allowed energy eigenstates for electrons in the conduction band (CB) and holes in the valence band (VB). The requirement for momentum conservation during photon emission means that a direct-gap semiconductor (e.g. GaAs) – in which the top of the VB and bottom of the CB have the same wave vector in the Brillouin zone – typically emits light much more efficiently than an indirect-gap semiconductor (e.g. Si). Changing the crystal structure of a semiconductor can radically alter its band structure, providing new opportunities to engineer device-critical properties (a concept known as crystal phase engineering).

It has remained a persistent challenge to develop green-wavelength ( $\lambda$  - 550 nm) emitters for a range of applications, with the lack of suitably efficient light-emitting materials in this spectral range constituting the so-called "green gap" for LED technology. While GaP is indirect-gap in its conventional zinc blende phase (left-hand figure), it is direct-gap in its wurtzite phase (right-hand figure), raising the possibility of enhanced efficiency for radiative recombination. Wurtzite GaP has predicted band gap energy Eg - 2.25 eV, corresponding to green-wavelength emission ( $\lambda$  = hc/Eg - 550 nm). It is therefore of strong interest to develop a detailed understanding of light emission from wurtzite GaP. This project in computational materials physics will address this problem by establishing predictive calculations of the wurtzite GaP band structure and radiative recombination rate.





#### Methods:

The project will begin with first principles band structure calculations, based on density functional theory. Band structures will be benchmarked vs. literature data, and used as input to compute spontaneous emission spectra to provide quantitative insight and facilitate comparison to experiment. The intern will receive training through research in the application of density functional theory, will acquire hands-on experience in scientific computing, and will develop an understanding of the optoelectronic properties of semiconductors.

#### Predicted results and impact:

The aim of this project is to establish predictive calculations of radiative recombination in wurtzite GaP. The outcome will be an enhanced understanding of the implications of wurtzite-phase band structure for optical emission, providing a quantitative assessment of wurtzite GaP as a green-wavelength emitter.

#### References:

L. H. Galvão Tizei and M. Amato "Electronic structure and optical properties of semiconductor nanowires polytypes", Eur. Phys. J. B 93, 16 (2020). DOI: 10.1140/epjb/e2019-100375-7

Location: Tyndall Type: Hybrid

Key words: III-V semiconductors, photonics, crystal phase engineering, density functional theory

Degree(s) that will suit this project: physics

## Generative Design of Integrated Photonic Filters

Theme: Monolithic & Heterogeneous Integrations

III-V Materials

Supervisor: Abi Waqas Co-Supervisor: Brian Corbett



#### Background:

Silicon photonics is a promising platform for photonic ICs due to its high integration density, low waveguide losses and compatibility with CMOS processes. Various ultra-compact silicon photonic devices, including active and passive components, have been developed successfully for various applications. Among the passive components, photonic filters are one of the most important elements, as they are used for spectral manipulation in optical systems. The current process of designing photonic filters is manual and time-consuming, requiring filter designers to have a deep understanding of the design process. This project will develop an algorithm that uses a computeraided design (CAD) tool to automate the design process. This will make the process much faster and easier, and it will also allow for more accurate designs without the need for specialized design knowledge. This project aims to develop a technology independent automated design tool for integrated photonic filters. The tool will take the user's filter requirements as input and generate an optimized design as output. The tool will be based on a generative design approach, which uses algorithms to explore and generate a variety of designs, and then selects the best design based on the user's requirements. The tool will be able to design cascaded filter structures based on Mach-Zehnder interferometers (MZIs), micro-ring resonators (MRRs) and ring- loaded Mach-Zehnder interferometer.

#### Methods:

- Develop an algorithm to generate filter designs (cascaded FIR, IIR, or hybrid) based on filter specifications provided by the user. Python or MATLAB scripts will be used to implement the algorithm.
- Develop a script to automatically generate simulation setups based on the design parameters obtained from the algorithm.
- · Analyse and optimize the filter designs to meet the specified requirements.
- (Optional) Fabricate prototype filters using available resources.
- (Optional) Perform experimental validation by comparing the fabricated filters with simulations and specifications.

- A functional algorithm for optimized photonic filter design and simulation setups meeting specified requirements.
- The development of skills in intern to use advanced photonic design tools and techniques, as well
  as teamwork and communication.

The predicted impact of this project is to streamline the filter design process, reduce manual efforts, and enhance the efficiency of filter optimization in the field of photonic engineering.

#### References:

Madsen, C. K., & Zhao, J. H. (1999). Optical filter design and analysis: a signal processing approach.
 Filter Design." MATLAB & Simulink, www.mathworks.com/discovery/filter-design.html.
 Accessed 4 Nov. 2023.

[3] Optical Filters - Ansys Optics, optics.ansys.com/hc/en-us/articles/360042323534-Optical-filters. Accessed 4 Nov. 2023.

Location: Tyndall Type: Hybrid

Key words: Photonic Integrated Circuits, FIR Filter, IIR Filter, Wavelength Division Multiplexor,

Generative Filter Design

Degree(s) that will suit this project: Physics and Engineering

#### **Automatic Thermal Tuning of** PICs to Reconfigure and Achieve Wavelength Locking

Theme: Monolithic & Heterogeneous Integrations

III-V Materials

Supervisor: Abi Wagas Co-Supervisor: Brian Corbett



#### Background:

Photonic integrated circuits (PICs) are evolving towards reconfigurable architectures and programmable photonic processors, which enable the implementation of many different functionalities on-demand [1]. These schemes rely on many optical interferometers, such as Mach-Zehnder interferometers (MZIs) and microring resonators (MRRs), which are sensitive to the phase delay between the interfering optical beams. For example, the delay line architecture proposed in [2] requires many thermal controllers to control the device's delay and operating frequency to match the incoming signal's frequency. Additionally, phase perturbation can substantially affect the PIC's performance. Phase perturbations are naturally caused by fabrication process tolerances. Temperature changes caused by environmental thermal fluctuations or on-chip heat sources can also cause time-varying phase drifts [3]. Actuators are required to actively control the phase in optical waveguides to compensate against phase errors and reconfigure and stabilize the PIC's working point. Thermal actuators are a well-established approach, but they can cause mutual thermal crosstalk between neighbouring actuated waveguides, which can impair the efficiency of PIC tuning and stabilization. In this project, we deploy a method for tuning and wavelength locking of PICs in conjunction with a technique to cancel the effects of thermal crosstalk in arbitrary PICs [4]. We will achieve this goal by performing numerical simulations and experiments on cascaded MZI based delay lines [2] where usually the number of controllers is in order of tens.

#### Methods:

- · Develop and implement a tuning algorithm to reconfigure and wavelength lock delay lines using existing tools.
- . Use Thermal Eigenmode Decomposition [4] to cancel the effects of thermal crosstalk in the developed algorithm.
- · Perform numerical simulations by actively tuning and configuring the delay line, with reduced thermal crosstalk effects to guarantee reliable control and high performance.
- Experimentally validate the method by reconfiguring and wavelength locking delay lines.

We will implement a tuning algorithm to reconfigure and wavelength lock delay lines, with reduced thermal crosstalk effects. While we will use delay lines as a demonstration circuit, the algorithm will be applicable to arbitrary PICs and can be used by other members of the IPIC. Additionally, the project will give interns real-world experience in characterizing complex photonic circuits and using CAD tools for real-world applications. This experience will be valuable to interns as they pursue careers in the field of photonics.

#### References:

- Pérez-López, et al (2020). Multipurpose self-configuration of programmable photonic circuits.
   Nature communications, 11(1), 6359.
- [2] Waqas, A., et al (2018). Cascaded Mach-Zehnder architectures for photonic integrated delay lines. IEEE Photonics Technology Letters, 30(21), 1830-1833.
- [3] Waqas, A., et al (2018). Stochastic process design kits for photonic circuits based on polynomial chaos augmented macro-modelling. Optics express, 26(5), 5894-5907.
- [4] Milanizadeh et al (2019). Cancelling thermal crosstalk effects in photonic integrated circuits. Journal of Lightwave Technology, 37(4), 1325-1332.

Location: Tyndall Type: In-person

Key words: delay line, control algorithms, integrated photonics, phase coupling, thermal cross talk, tuning and wavelength locking

Degree(s) that will suit this project: Physics and Engineering

### High efficiency red emitting LEDs

Theme: Monolithic & Heterogeneous Integrations

III-V Materials

Supervisor: Ning Liu

Co-Supervisor: Brian Corbett





#### Background:

High efficiency light-emitting diodes (LEDs) are based on blue emitters with phosphor down-conversion and since their introduction have changed the way that general lighting and displays are implemented. The next generation of LEDs will use separate red-green-blue for higher contrast and more energy efficient displays. However, red LEDs based on InGaP alloys suffer severely from inefficiencies as the dimensions of the LED are reduced due to surface recombination. Hence, an effective method to passivate the surfaces of the semiconductor alloys is urgently needed. In this project we want to compare different passivation techniques using organic and inorganic means and to compare the results with LEDs based on upcoming InGaN based materials. The project will be primarily based at the University of Limerick and the work will be in collaboration with Tyndall. Ideally the researcher will be based in UL and visit Tyndall on a number of occasions. A chemistry background is beneficial.

#### Methods:

- Background study on physics of recombination in LEDs
- · Plan experimental matrix
- · Prepare LED materials
- Passivate with different methods (Liquid, gas and atomic layer deposition)
- Characterise passivated materials using fluorescence microscopy and carrier lifetime measurements
- · Compare with red materials based on GaN
- · Analysis and summary

#### Predicted results and impact:

Breakthrough in efficiency of small sized red LEDs

#### References:

Micro-Light Emitting Diode: From Chips to Applications, Peter J. Parbrook, Brian Corbett, Jung Han, Tae-Yeon Seong, Hiroshi Amano Background:

Location: University of Limerick

Type: In-person

Key words: LEDs, displays, red emitters, surface passivation Degree(s) that will suit this project: Physics, engineering

#### Data Communication with Visible Light Emitting Diodes

Theme: Monolithic & Heterogeneous Integrations

III-V Materials

Supervisor: Zhi Li

Co-Supervisor: Brian Corbett



#### Background:

Information flow is the bottleneck in modern communication systems and so every means to increase the data transfer is valuable. Light-emitting diodes (LEDs) operating across the visible spectrum are now being investigated for high bandwidth low cost communications under the general headings of Visible light Communication (VLC) or LiFi. This is because LEDs, unlike lasers, do not have a threshold, can easily be made into 2 dimensional arrays and are low cost. In addition, LEDs based on GaN materials are robust at high temperature meaning that they can be integrated directly with silicon circuitry. However, the recombination time in LEDs is longer than in lasers limiting the bandwidth and the light is divergent. In this project, we will study a variety of LEDs to measure and compare their bandwidth. LEDs emitting at different wavelengths and with different sizes will be investigated.

#### Methods:

- . Background study on properties of LEDs
- Characterise LED devices for light, current, voltage
- · Set-up data communication measurement
- Characterise LEDs in free space and with glass waveguides
- Analyse data and present results

#### Predicted results and impact:

- · Familiarize the set-ups of using LEDs for communications
- Understand the bandwidth properties in LEDs made of different materials/chip sizes
- Hasten the introduction of Visible Light Communications

#### References:

- 1.Transfer printing of roughened GaN-based light-emitting diodes into reflective trenches for visible light communication, Z Shaban, Z Li, B Roycroft, M Saei, T Mondal, B Corbett, Advanced Photonics Research 3 (8), 2100312 (2022): Background:
- 2. https://lifi.co/visible-light-communication/
- 3.GHz bandwidth semipolar (112 2) InGaN/GaN light-emitting diodes, Optics letters 41 (24), 5752 https://cora.ucc.ie/items/de099016-0788-4bf4-8045-1b46b53c3724

Location: Tyndall

Type: In-person

Key words: LEDs, VLC, and communication

Degree(s) that will suit this project: Physics, Engineering

#### Advanced Digital Signal Processing Design Enabling Future Optical and Wireless Access

Theme:

Optical Communications

Supervisor:

Xing Ouyang



#### Background:

Towards 2030s and beyond, Europe and the world will embrace unprecedented opportunities whilst facing grand challenges of growth and sustainability of the globe. Wireless technologies have profound impact on our modern society and economy, as well as our daily life. Especially, along with the rollout of 5G networks since 2020, the continued technological evolution towards 6G, which will be expected to be deployed in the 2030s, will be strategically important to the societal and economic opportunities and challenges of the post-Pandemic world.

In response to the needs for 6G in the 2030s, research and innovation initiatives are being proactively kicked off globally [1]. People are exploring novel communication technologies, such as, new signal modulation, medium access techniques, optical/wireless convergence, and system structures. Signal modulation is crucial that directly determines signal quality, efficiency of spectral usage, resilience to impairments from the system and radio channels and interference from other wireless users.

#### Methods:

In this project, we will specifically study advanced physical layer modulation technologies enabling the air interface for future optical & wireless networks. These technologies include orthogonal frequency-division multiplexing (OFDM) [2], and the emerging orthogonal chirp-division multiplexing (OCDM) [3], as well as enabling digital signal processing (DSP) techniques based on simulation and we will base on the software defined radio (SDR) or field program gate array (FPGA) platforms to investigate cutting-edge algorithms.

Specifically, the student is expected to have a high-level design of the baseband modulation based on OFDM or OCDM, i.e., the transmitter that includes information source generating bit stream, symbol modulation using quadrature amplitude modulation (QAM), waveform modulation using fast Fourier transform/fast Fresnel transform, and digital-to-analog conversion; the receiver performs reversal operations to recover the information. The design will be implemented based on both numerical simulation for performance study and experiment testbed for hardware validation. The devised algorithms be programmed into hardware design language in either VHDL or Verilog based on Xilinx field program gate array (FPGA) VIVADO® platform, using one of the following boards: Kintex-7 evaluation board (kc705), Virtex-7 UltraScale (VCU108), the system-on-module based on Analog Devices ADRV9361-Z7035 or Adalm-Pluto Software Defined Radio available in the lab.

The predicted results should include high level design of OFDM/OCDM systems, behaviour-level, register transfer level design of the systems, and the validation and simulation model, and finally the hardware demonstration of the validated design.

#### References:

- S. Dang, O. Amin, B. Shihada, and M.-S. Alouini, "What should 6G be?," Nature Electronics, vol. 3, no. 1, pp. 20-29, Jan. 2020, doi: 10.1038/s41928-019-0355-6.
- [2] S. B. Weinstein, "The History of Orthogonal Frequency-Division Multiplexing," (in English), IEEE Commun Mag, Article vol. 47, no. 11, pp. 26-+, Nov 2009, doi: Doi 10.1109/Mcom.2009.5307460.
- [3] X. Ouyang and J. Zhao, "Orthogonal chirp division multiplexing," IEEE T Commun, vol. 64, no. 9, pp. 3946–3957, Jul. 2016, doi: 10.1109/TCOMM.2016.2594792.

Location: Tyndall

Type: In-person

Key words: Wireless communications, fibre-optic systems, digital signal processing, software defined radio, FPGA, Verilog, MATLAB.

Degree(s) that will suit this project: electrical engineering/computer science

#### Software Defined Radio Implementation for High-Speed Systems

Theme:

Optical Communications

Supervisor:

Xing Ouyang

#### Background:

Towards 2030s and beyond, Europe and the world will embrace unprecedented opportunities whilst facing grand challenges of growth and sustainability of the globe. Wireless technologies have profound impact on our modern society and economy, as well as our daily life. Especially, along with the rollout of 5G networks since 2020, the continued technological evolution towards 6G, which will be expected to be deployed in the 2030s, will be strategically important to the societal and economic opportunities and challenges of the post-Pandemic world.

In response to the needs for 6G in the 2030s, research and innovation initiatives are being proactively kicked off globally [1]. People are exploring novel communication technologies, such as, new signal modulation, medium access techniques, optical/wireless convergence, and system structures. Signal modulation is crucial that directly determines signal quality, efficiency of spectral usage, resilience to impairments from the system and radio channels and interference from other wireless users.

#### Methods:

In this project, we will specifically study advanced physical layer modulation technologies enabling the air interface for future optical & wireless networks. These technologies include orthogonal frequency-division multiplexing (OFDM) [2], and the emerging orthogonal chirp-division multiplexing (OCDM) [3], as well as enabling digital signal processing (DSP) techniques based on simulation and we will base on the software defined radio (SDR) or field program gate array (FPGA) platforms to investigate cutting-edge algorithms for next-generation mobile networks.

Specifically, the student is expected to have a high-level design of the baseband modulation based on OFDM or OCDM, i.e., the transmitter that includes information source generating bit stream, symbol modulation using quadrature amplitude modulation (QAM), waveform modulation using fast Fourier transform/fast Fresnel transform, and digital-to-analog conversion; the receiver performs reversal operations to recover the information. The design will be implemented based on both numerical simulation for performance study and experiment testbed for hardware validation. The devised algorithms be programmed into hardware design language in either VHDL or Verilog based on Xilinx field program gate array (FPGA) VIVADO® platform and using the advanced SDR platform USRP-X310 from National Instrument.

The predicted results should include high level design of OFDM/OCDM systems, behaviour-level, register transfer level design of the systems, and the validation and simulation model, and finally the hardware demonstration of the validated design.

#### References:

- [1] S. Dang, O. Amin, B. Shihada, and M.-S. Alouini, "What should 6G be?," Nature Electronics, vol. 3, no. 1, pp. 20-29, Jan. 2020, doi: 10.1038/s41928-019-0355-6.
- [2] S. B. Weinstein, "The History of Orthogonal Frequency-Division Multiplexing," (in English), IEEE Commun Mag, Article vol. 47, no. 11, pp. 26-+, Nov 2009, doi: Doi 10.1109/Mcom.2009.5307460.
- [3] X. Ouyang and J. Zhao, "Orthogonal chirp division multiplexing," IEEE T Commun, vol. 64, no. 9, pp. 3946–3957, Jul. 2016, doi: 10.1109/TCOMM.2016.2594792.

Location: Tyndall Type: In-person

Key words: Wireless communications, fibre-optic systems, digital signal processing, software defined radio, FPGA, Verilog, MATLAB.

Degree(s) that will suit this project: electrical engineering/computer science

# Distributed Sensing Using Rayleigh Scattering in Optical Fiber

Theme: Optical Communications

Supervisor: Conor Russell Co-supervisor: Cleitus Antony



#### Background:

Rayleigh scattering in optical fibers is the result of density fluctuations (scatterers) within the fiber core caused by the manufacturing process. The light scattered by the density fluctuations is the predominant source of attenuation in optical fiber transmission. This fiber impairment can, however, be leveraged to transform a standard optical fiber into a distributed sensor than can be tens of kilometres long.

By observing the Rayleigh backscattering from a short optical pulse as it propagates through the fiber, measurements can be mapped to specific locations within the fiber based on the pulses time of flight. This is a technique known as optical time domain reflectometry (OTDR). OTDR is commonly used to monitor optical networks for fiber breaks or abnormal attenuation.

A modification of OTDR known as phase sensitive OTDR (φ-OTDR) can be achieved by using narrow linewidth laser sources in OTDR. This allows for the observation of coherent interference between the light scattered by different scatterers within the pulse. Interference occurs due to the position related phase difference between scatterers. The position of scatterers within the fiber is sensitive to external strains applied to the fiber. Therefore, the interference between scatterers can be used to locate and measure strain applied to the fiber.

Many innovations in  $\phi$ -OTDR have come from the adoption of using optical communications techniques and technologies in a distributed sensing context. This has led to  $\phi$ -OTDR systems using many of the same components as a communications system. A prime example of this is the change from direct detection receivers to coherent receivers in  $\phi$ -OTDR. Direct detection can only provide intensity measurements which can be used to locate changes in strain but are not suitable for quantitative measurement of strain magnitude. The use of coherent detection, however, allows the phase of the backscattered light to be measured.

In recent years there has been increased interest in the integration of  $\phi$ -OTDR to existing optical communications network transceivers. This would allow for the deployed fiber infrastructure to act as a sensor that could have applications in Structural Health Monitoring, traffic monitoring, intrusion detection and pre-emptive fault monitoring of the fiber network.

#### Methods:

The work will be carried out in the state-of-the-art photonic systems lab in Tyndall National Institute The student will work with MATLAB programming tools for analysis of experimental data.

The predicted result is an experimental comparison of direct detection and coherent detection φ-OTDR performance. This project will provide experience in characterisation of distributed sensing systems and the use of optical devices essential to both sensing and optical communications.

#### References:

- [1] Ip, E, et al., 2021. 'Distributed fiber sensor network using telecom cables as sensing media: technology advancements and applications [Invited]'. Journal of Optical Communications and Networking, 14(1), p.A61.
- [2] Cantono, M., et al., 'Optical Network Sensing: Opportunities and Challenges', OFC 2022, M2F.1
- [3] Z. Pan, K. Liang, Q. Ye, H. Cai, R. Qu, and Z. Fang, "Phase-sensitive OTDR system based on digital coherent detection," Optical Sensors and Biophotonics, 2011.

Location: Tyndall Type: In-person

Key words: Phase sensitive OTDR, coherent detection, direct detection

Degree(s) that will suit this project: Engineering (Computer, Electronics, related), Physics,

Mathematics

# Smart insect monitoring in orchards using deep learning (DL) models on smart mobile phones and Raspberry Pi

Theme: Smart Systems
Supervisor: Amin Kargar
Co-Supervisor: Brendan O'Flynn



#### Background:

Approximately 40% of all crops are destroyed by pests, resulting in a loss of \$220 billion worldwide [1]. An effective insect monitoring system is essential for reducing this loss and sustainable agriculture. In this regard, traditional methods for insect monitoring in the field are labor-intensive and time-costly, and often need a high level of entomological knowledge [2]. However, advancements in technology, particularly in the field of deep learning and computer vision, offer the potential to revolutionize insect monitoring by enabling the automation of data collection and analysis [3].

This proposal focuses on the development and implementation of a Deep Learning (DL) object detection/segmentation/counting model for insect monitoring in agricultural orchards. The model will be deployed on cost-effective and portable devices, such as the Raspberry Pi and smart mobile phones, making it accessible to a wide range of users, including small-scale farmers. The primary objectives of this project are to develop an accurate insect detection/segmentation/counting model, integrate it into user-friendly applications, and assess its impact on insect monitoring in agricultural contexts.

This proposal is divided into two main parts, each focusing on specific aspects of the proposal for two different individuals to work on. By dividing the proposal into two parts, two individuals can work on their respective sections and ensure that all necessary details are covered.

#### Methods:

#### Part 1:

Title: Insect monitoring in orchards using deep learning (DL) based models on smart mobile phones and Raspberry Pi with focus on Deep Learning model designing

#### Method:

Literature Review:

Summarize the relevant research on deep learning models for insect detection/segmentation/counting.

#### Dataset preparation:

Gather a diverse dataset of images of insects commonly found in agricultural fields. Annotate the dataset with bounding boxes to identify and label insects of interest.

#### DL Model Development:

Detail the training process of deep learning models, including the choice of architectures and transfer learning techniques. Train a deep learning object detection model using state-of-the-art architectures with transfer learning. Fine-tune the model on the insect-specific dataset to improve accuracy and reduce false negatives and false positives.

#### Part 2:

Title: Insect monitoring in orchards using deep learning (DL) based models on smart mobile phones and Raspberry Pi with focus on implementing user-friendly applications on Raspberry Pi and Smart Mobile Phones

Method:

Literature Review:

Summarize the relevant research on insect monitoring and the use of portable platforms like Raspberry Pi and Android/iOS devices.

Application Development:

Develop user-friendly applications for both Raspberry Pi and Android/iOS mobile phones that integrate the trained insect detection model with a focus on real-time processing and data transferring, storage, and visualization features for insect monitoring.

#### Predicted results and impact:

Results: The deep learning model is expected to achieve a high level of accuracy in detecting/classifying/counting insects. The applications developed for Raspberry Pi and Smart mobile phones should provide fast and efficient processing of insect images and videos users should find the applications easy to use, with intuitive features for data storage and visualization.

Impact: The implementation of this technology is expected to significantly reduce the time and effort required for insect monitoring in agricultural fields. The project's success will empower farmers and agricultural experts to make more informed decisions regarding pest management, helping to reduce crop losses and increase yields.

#### References:

- FAO Climate change fans spread of pests and threatens plants and crops, new FAO study, 2 June 2021,
- [2] van Klink, Roel, Tom August, Yves Bas, Paul Bodesheim, Aletta Bonn, Frode Fossøy, Toke T. Høye et al. "Emerging technologies revolutionise insect ecology and monitoring." Trends in ecology & evolution (2022).
- [3] Preti, Michele, François Verheggen, and Sergio Angeli. "Insect pest monitoring with cameraequipped traps: Strengths and limitations." Journal of pest science 94, no. 2 (2021): 203-217.

Location: Tyndall

Type: In-person

Key words: Smart Insect Monitoring, Smart Agriculture, Deep Learning, Object Detection, Python, Mobile Applications (Android or iOS)

Degree(s) that will suit this project: Engineering (Computer, Electronics, related)

#### Design, Testing, and Validation of RF Front-end Components for Emerging Communications



Theme: Wireless RF communications

Supervisor: Dimitra Psychogiou Co-Supervisor: Steven Matthew Cheng

#### Background:

The continuous and rapid growth of wireless communications demands radio frequency (RF) frontend systems able to support multiple standards and applications while exhibiting low size, weight
and power (SWaP). Multi-functionality in the RF front-end is typically incorporated by adding
dedicated RF front-end chains for every application and standard and switching between them using
a large number of switches. As a matter of fact, they become really large, complex and power hungry
due to being based to a large number of static RF components. By incorporating RF tuning and by
combining multiple RF signal processing functions into a single RF component, SWaP can be greatly
reduced. As such, recent research efforts are focusing on the realization of highly integrated multifunctional and multi-configurable RF circuits/components for the miniaturization of RF transceivers.
This project aims to develop tuning methods for RF co-designed filters and active components such
as low noise amplifiers to form a highly-integrated multifunctional RF component that supports
multiple levels of transfer function adaptivity and reconfigurability.

#### Methods:

In this project, RF circuit-based co-design techniques will be investigated for the realization of compact RF components using circuit-based simulators (e.g ADS Keysight) and full-wave electromagnetic analysis software (e.g ANSYS HFSS). The project will also investigate RF methodologies using semiconductor-based variable capacitors and mechanical actuators alongside effective tuning algorithms that facilitate quick and autonomous RF tuning using machine learning. Machine learning algorithms tailored to reconfigure physical parameters of the RF component in response to multiple RF performance parameters will be developed. The intern is expected to assist in the design, testing, and validation of these RF components and algorithms.

#### Predicted results and impact:

This work is in line with the overarching goal of investigating and designing novel RF front-end components for emerging and future communication systems. By working on this project, the intern gets to familiarize with both theoretical and experimental work involving RF components and circuits.

#### References:

[1] K. Zhao and D. Psychogiou, "Monolithically integrated coaxial resonator-based filtennas using SLA 3D printing," IEEE Antennas and Wireless Propagation Letters, Vol. 22, No. 1, pp. 189 - 193, Jan. 2023.

[2] J. A. Estrada, S. Johannes, D. Psychogiou and Z. Popović, "Tunable Impedance-Matching Filters," in IEEE Microwave and Wireless Components Letters, vol. 31, no. 8, pp. 993-996, Aug. 2021, doi: 10.1109/LMWC.2021.3083184.

[3] A. Ashley and D. Psychogiou, "Ferrite-based multi-port circulators with RF co-designed bandpass filtering capabilities," IEEE Trans. Microw. Theory Techn, Vol. 71, No. 6, pp. 2594-2605, January 2023.

[4] M. F. Hagag, M. Abu Khater and D. Peroulis, "Balanced-Balanced Tunable Filtering LNA using Evanescent-Mode Resonators," 2019 IEEE MTT-S International Microwave Symposium (IMS), Boston, MA, USA, 2019, pp. 13-16.

Location: Tyndall Type: In-person

Key words: co-design, filters, radio frequency, reconfigurable.

Degree(s) that will suit this project: Engineering, Computer Science, Math, and Physics degrees.

Preferred: have an understanding of circuit analysis (linear and non-linear), semiconductor devices, machine learning, python.

## Development of an Innovative Modelling Tool for Advanced Wirelessly Powered **Biomedical Implants**



Wireless RF communications & MCCI Theme:

Supervisor: John Buckley Co-Supervisor: Daniel O'Hare



#### Background:

In this work, an innovative electromagnetic model has recently been developed to rapidly compute the amount of radio frequency (RF) power that can be delivered to a highly integrated wirelessly powered implant in medical applications (Figure 1 (a) and (b)) [1]. This is a highly innovative model that can compute in seconds versus hours using traditional finite element (FEM) models. Our goal now is to bring this model to the next level and add an intuitive and easy to use graphical user interface (Figure 1 (c)). This will enable the user to easily and rapidly model different wirelessly powered implantable medical devices and will be the first of its kind.

#### Methods:

The student will learn to simulate our current model using MATLAB. The student will then use their creativity to develop an exciting graphical user interface (GIU) to interface with the current MATLAB model. The model is intended to be published and used by international researchers and will need to be captivating to use and provide easy to interpret results.

#### Predicted results and impact:

The goal is to make the developed model available internationally, to the research community worldwide to enable ground-breaking research in wireless bio-implantable sensor applications.

#### References:

[1] Brendan O'Callaghan, Dinesh R Gawade et al., "A Time-Efficient Model for Estimating Far-Field Wireless Power Transfer to Biomedical Implants" IEEE EuCAP-2024, under review

Location: Tyndall Type: In-person

Key words: Wirelessly Powered Implantable Medical Devices, Electromagnetics

Degree(s) that will suit this project: Electrical/Electronic Engineering, Computer Science with focus

on programming in MATLAB and Python