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SUMMER FELLOWSHIP PROGRAMME 2025 PROJECT DESCRIPTIONS

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Development and application of Machine Learning Potentials for Novel Functional Materials.

Theme: CMOS & Emerging Platforms
Supervisor: Michael Nolan
Co-Supervisor: James Brown

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Background:
Atomistic simulations using density functional theory and molecular dynamics are routinely used in discovering and understanding materials, chemistries and processes to produce functional thin films. The Materials Modelling for Devices Group at Tyndall is at the forefront of this work with applications in semiconductor devices, catalysts for removal of pollutants, materials processing and discovering sustainable materials, e.g. replacement of fluorine-containing chemicals.
The cost of simulations is significant requiring days to months to complete a calculation, even on high performance computing systems. Machine learning, that is built on available simulation data, is established as an approach to rapidly screen materials and chemistries to explore a wider chemical space and arrive at useful candidate materials – essentially it can provide a filtering approach where rapid ML simulations can filter out undesired options, leaving a small number for deeper investigation.
The aim of this Fellowship is to work with members of the group to take their atomistic simulation data and outputs and train a machine learning potential that can deliver accurate simulation data on a wider range of materials and chemistries thus allowing candidate materials to be chosen. The targeted applications include:

- Prediction of metal deposition on metal nitrides and 2D materials for semiconductor devices
- Prediction of novel ferro- and piezoelectric materials and the role of defects
- Prediction of non-fluorinated chemicals for materials processing and non-fluorinated materials for tribology.

Methods:
First principles simulations using state of the art first principles density functional theory (DFT) are being used within the host group for novel materials discovery on high performance computing infrastructure. This yields the structure, stability and relevant chemical properties of target materials to predict their performance. Unfortunately, this powerful and crucial approach to materials development is limited by the time and computing resources needed for full DFT calculations. The DeepMD neural network potential method that will be deployed in this Fellowship will use these DFT data as training data to produce new neural network potentials that can be used to rapidly compute relevant properties of candidate materials - ca. 2 minutes compared to days for DFT so that thousands of structures can be rapidly assessed. Coding is required as part of the training, validation and deployment of the potentials.

Predicted results and impact:
Using existing (and new data as needed) DFT results for materials are used to train new neural network potentials to enable simulation of structures with thousands of atoms, including (i) simulation of defects, (ii) simulation of complex surface chemistries and reactivity and (iii) longer timescale simulations. This will also deliver new ML models for wider use within the group. A key impact is the training of the Fellow on advanced simulation tools and applications in real materials as well as wider transferable skills development.

References:

1. https://docs.deepmodeling.com/projects/deepmd/en/r2/index.html,
2. https://www.sciencedirect.com/science/article/pii/S0010465518300882,
3. https://link.aps.org/doi/10.1103/PhysRevLett.120.143001,
4. https://pubs.aip.org/books/monograph/137/book-pdf/12805891/9780735425279.pdf#page=116,
5. https://journals.aps.org/prb/abstract/10.1103/PhysRevB.107.224301

Location: Tyndall

Type: Hybrid, min 3 days in person

Key words: Machine learning, Python, Catalysts, Metal Oxides, Deposition, Materials

Degree(s) that will suit this project: Materials Science, Chemistry, Physics, Theoretical Physics, Chemical Physics.

Exploring Topological Structures in a Room-Temperature Multiferroic Material for Future Data Storage

Theme: CMOS & Emerging Platforms
Supervisor: Lynette Keeney
Co-Supervisor: Joydipto Bhattacharya

Tyndall National Institute
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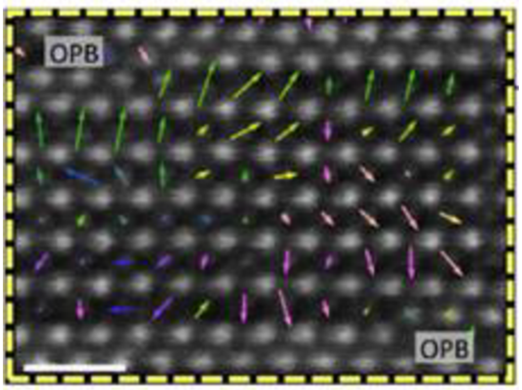
Background:
The increase in data generation due to remote learning, online work, and digital entertainment is extraordinary. To visualize this, in 2013, the global data usage could have been represented as a stack of smart tablets that would stretch two-thirds of the way to the Moon. By 2025, this data stack could reach the Moon and back over 26 times! This massive growth presents challenges, not only in how we store such large amounts of data but also in processing it quickly.



This project focuses on an exciting type of structure in materials called polar vortices. Polar vortices are swirling patterns of electric polarization, similar to magnetic "spin whirlpools" known as skyrmions. Recently, researchers have discovered polar vortices in ferroelectric materials, and these are considered a major breakthrough for next-generation electronics because they could lead to new ways of storing data beyond what traditional methods can achieve.[1] However, there's still a lot to learn about how these polar vortices form and how we might create them on demand.

Multiferroic materials, which have both ferroelectric (electric) and ferromagnetic (magnetic) properties, are particularly promising for this research.[2] However, these materials are rare, and studying how their electric and magnetic behaviours work together in topological structures is still in the early stages.[3]
Dr Keeney's group has recently discovered unique structures, like charged domain walls and polar vortices, in a multiferroic material.[4] The goal of this project is to understand these structures better and to develop new ways to design and predict them for future applications, such as neuromorphic (brain-inspired) computing and quantum computing.

Methods:
This project will primarily focus on theoretical work, but the Summer Fellow will also have opportunities to engage in practical, hands-on activities. During this time, the Summer Fellow will learn and apply the following techniques:
Density Functional Theory: a computational method used to model and understand the properties of materials on an atomic level.

Thin-Film Deposition: a technique for creating ultra-thin layers of material, which is essential for developing advanced electronic devices.

Scanning Probe Microscopy: a method for examining surfaces and structures at the nanoscale, allowing detailed study of material properties.
This combination of theoretical modelling and practical lab techniques will provide the intern with valuable skills for research in materials science.

Predicted results and impact:
This research will provide valuable hands-on experience for the fellow, enhancing their CV. By advancing our understanding of these unique materials and optimising how they are grown, this work could contribute to the development of ultra-compact, low-power memory storage solutions. Such technology might eventually be used in neuromorphic computing and quantum computing, where energy-efficient, advanced data storage is key.

References:

1. https://doi.org/10.1063/5.0034914
2. https://doi.org/10.1111/jace.12467
3. https://doi.org/10.1021/acs.chemmater.4c00413
4. https://doi.org/10.1021/acsami.1c17383

Location: Tyndall

Type: Fully In-person

Key words: Materials, Ferroelectrics, Multiferroics, Domain Walls, Topological Structures.

Degree(s) that will suit this project: Physics, Chemistry, Chemical Physics, Material Sciences, Mathematics, Computer Science.

Sensor interfaces using Time based circuits

Theme: CMOS & Emerging Platforms
Supervisor: Daniel O'Hare

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Background:
New sensors to detect viruses, DNA and other micro-organisms are becoming more popular. Many of these biosensors yield an output current proportional to their stimulus, with examples including electrochemical sensors, photodiodes, Nanopore sensors, ISFETs etc. Furthermore, in lab-on-chip applications it is desired to have multiple sensors and multiple readout channels in parallel. To this end, we have invented a low area, low power, single-ended current-to-digital converter (CDC) [1] which can be used in an array to readout multiple biosensors in parallel. Presently we have a single channel readout prototype, we want a student to work with us on an array readout.

Methods:
The intern will learn to simulate our current to digital converter using Cadence simulation tools. They will also get to work on the physical design (layout) of the circuits. There will also be opportunities to test our prototype devices with different sensors such as photodiodes and resistive sensors.

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 industry standard tools such as Cadence and they will learn about the applications that are enabled by sensors producing current signals.

References:

1. A. Wall, P. Walsh, K. Sadeghipour, I. O'Connell and D. O'Hare, "An Improved Linearity Ring Oscillator-Based Current-to-Digital Converter," in IEEE Solid-State Circuits Letters, vol. 5, pp. 202-205, 2022, doi: 10.1109/LSSC.2022.3198367.
2. A. Wall, P. Walsh and D. O'Hare, "A Model & Design Methodology for Dead Time Linearised Current Controlled Ring Oscillator ADCs," in IEEE Transactions on Circuits and Systems II: Express Briefs, doi: 10.1109/TCSII.2024.3390216.

Location: Tyndall **Type**: Fully In-person

Key words: Integrated circuits, Sensor interface circuits, IC design, analogue

Degree(s) that will suit this project: Electronic engineering

Development of a single-mode tuneable fibre laser in the 2 µm waveband

Theme: Communications
Supervisor: Eoin Russell

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Background:
As the number a of photonic applications continues to grow and diversify, it is paramount that we develop new photonic technologies operating in novel wavelength ranges. In recent years the 2 µm waveband has sparked interest due to its potential to be utilised in the key fields of gas sensing, nonlinear silicon photonics and optical communications [1].
A key enabling technology for the above applications is a tuneable high power laser source. These tuneable lasers can produce light at a user selected wavelength, allowing for the agile testing of different optical systems and environments. Fibre lasers are of particular interest due to their potential to produce high optical power across a broad range of wavelengths. To produce optical emission in the 2 µm wavelength range, a Thulium or Thulium/Holmium doped fibre will be used as the laser gain material. Combining these gain materials with a suite of specialized 2 µm optical components will enable the production of single-mode laser emission across a wavelength range spanning over 250 nm [2]. Achieving single-mode lasing from such a device is nontrivial and requires careful control of many physical parameters in the system, including noise, polarisation, gain and loss. With careful design, these parameters can be tailored to produce a "pure" laser signal with high stability and low noise. The laser source developed in the project will be designed for applications in the nonlinear silicon photonic device characterisation.

Methods:
The project will consist of three key stages: design, construction and characterisation. During the design stage, the fundamental physics of fibre lasers will be studied, and a fibre laser design will be proposed. The laser source will then be constructed, and its performance will be studied in a cutting-edge laboratory setting.

Predicted results and impact:
The end result of this project will be a fully functional single-mode fibre laser operating in the 2 µm wavelength range. The characteristics of the laser source including power, tuning range, stability and noise will be optimised for application in the study of nonlinear silicon photonic devices.

References:

1. Russell, E. 2021. Technologies in the 2 µm waveband. PhD Thesis, University College Cork.
2. Z. Li, S. U. Alam, Y. Jung, A. M. Heidt, and D. J. Richardson, "All-fiber, ultra-wideband tunable laser at 2 µm," Opt. Lett. 38, 4739-4742 (2013)

Location: Tyndall

Type: Fully In-person

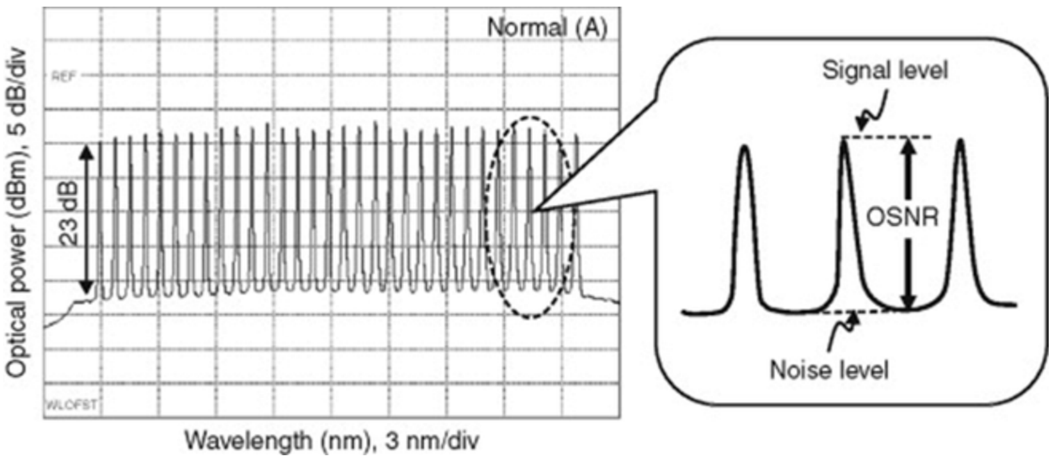
Key words: Fibre lasers, Fibre Amplifiers, Mid-IR photonics

Degree(s) that will suit this project: Physics, Maths & Physics, Applied Physics and Electronic Engineering

Optical Communications Telemetry Analysis

Theme: Communications
Supervisor: Fatima Gunning

Background:
Optical Communications is the science behind enabling the Internet, focusing on the infrastructure—especially ground-based systems—that supports both short- and long-distance communications. Current submarine systems employ 40 to 80 wavelength channels using a technique called Dense Wavelength Division Multiplexing (DWDM), as shown in Figure 1(a), achieving terabit-per-second capacities on a single fibre strand! This remarkable advancement introduces new challenges: with closely spaced wavelength channels for increased capacity, neighbouring channels often "overlap", making it difficult to distinguish each data stream. Long-distance transmission also suffers from loss, mitigated by optical amplifiers like Erbium-doped Fibre Amplifiers (EDFAs), which add noise, degrading signal quality. Additionally, dispersion and nonlinear effects must be monitored or compensated to ensure signal recovery.



One important monitoring tool, or telemetry tool, is the Optical Signal to Noise Ratio (OSNR), illustrated in Figure 1(b). OSNR measures the signal power on a specific wavelength channel divided by the noise present beneath the signal. Since EDFAs and other amplifiers introduce noise at the same wavelength as the signal, a lower OSNR indicates poorer signal integrity. In DWDM systems, close channel spacing makes noise measurement challenging, and each added amplifier increases noise accumulation. OSNR is thus vital for monitoring link-by-link and is typically measured with an optical spectrum analyser (OSA). OSAs, a type of spectrometer, offer high resolution (up to 10 pm) but are costly and slow, making it impractical to install them at every link for continuous DWDM channel monitoring.

Methods:

The idea here is to use a scanning Fabry-Perot filter of high finesse, electronics, in addition to signal processing, to build a compact and accurate OSNR measurement system that would replace the expensive OSAs.

The student will then use Python or any other alternative package to control the system and estimate the OSNR. Depending on the progress, the project can also analyse the potential of techniques such as machine learning and/or neural networks to accurately estimate the noise under the signal, depending on different conditions such as varied power levels of each channel, missing channels, amongst others.

Predicted results and impact:

The goals will be to:

1. Read relevant literature on: (a) OSNR and real time OSNR monitoring; (b) noise estimation based on a number of techniques;
2. Build and test compact OSNR measurement systems, comparing with OSA measurements;
3. Create a Python code that (a) captures optical spectrum traces; (b) analyse optical spectrum traces to capture wavelength channels; (c) and then captures signal power; (d) estimates noise;
4. Analysing the advantages and limitations of the cost-effective technique.

Real time OSNR monitoring can be difficult, and different methods have shown their pros and cons. By simplifying the acquisition system and utilising intelligent fast noise estimation algorithms, it is possible to eventually create photonic integrated circuits as chips that could be introduced anywhere in the network.

The work proposed here will hence have impact on the future optical networks topology, with the addition of simplified systems that can enable a true oversight of the entire network.

References:

1. Jun Haeng Lee, Yun C. Chung, Chapter 2 - Optical signal-to-noise ratio monitoring, from Optical Performance Monitoring, Academic Press, 2010, Pages 21-65. https://doi.org/10.1016/B978-0-12-374950-5.00002-X.
2. Brian Lavallée, Q&A with EXFO: Understanding Submarine OSNR, January 16, 2018 https://www.ciena.com/insights/articles/QA-with-EXFO-Understanding-Submarine-OSNR.html

Location: Tyndall

Type: Fully In-person

Key words: Optical communications, telemetry, OSNR estimation

Degree(s) that will suit this project: Physics

Silicon Front-End Components of Electronic-Photonic Integrated Wireless Communication System-On-Chips

Theme: Communications
Supervisor: Vaishnavi Jairam
Co-Supervisor: Vishal Jagtap

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Background:

Silicon based THz transceiver solutions are promising due to advantages such as low-cost robustness, hand-held capability, room temperature operation, and on-chip scalability. Within the context of developing silicon based fully integrated mm-wave terahertz transceiver system-on-chips for high-speed large bandwidth next generation 6G communication, we are seeking a Masters Summer Fellow to perform the literature review and evaluate the building blocks of silicon-based RF front-end components.

Methods:

The internship provides an opportunity to gain practical understanding of the implementation of state-of-the-art high-speed transistor technology in a system and hands-on experience on the latest CAD simulation tools and process development kit of the state-of-the-art silicon foundry processing technology. Following are the aims and objectives of the fellowship:

- Review of the state-of-the-art performances of RF front-end components for mm-wave – Terahertz system-on-chips.
- Simulate the basic RF/analogue circuit blocks using the high-speed transistors.
- Perform Data analysis using Python Jupyter Notebooks.
- Deliver periodic oral and written reports.

Predicted results and impact:

The fellow will have an opportunity to contribute to the ongoing innovative research project on electronic-photonic systems for high-speed large bandwidth wireless communications. The fellow will present the results within the institute's internal forums and will have the opportunity to be on the contributing authors' list for scientific publications.

References:

1. V. S. Jagtap, et al, "Monolithically Integrated Silicon Photodiodes For Terahertz Electronic-Photonic Integrated Systems," 2022 47th International Conference on Infrared, Millimeter and Terahertz Waves (IRMMW-THz), Delft, Netherlands, 2022, pp. 1-4, doi: 10.1109/IRMMW-THz50927.2022.9895657.
2. W. Jiang et al., "Terahertz Communications and Sensing for 6G and Beyond: A Comprehensive Review," in IEEE Communications Surveys & Tutorials, doi: 10.1109/COMST.2024.3385908.

Location: Tyndall

Type: Fully In-person

Key words: silicon, electronic-photonic integrated circuits, 6G wireless communication, terahertz technology, Millimeter wave communication,THz Communication

Degree(s) that will suit this project: Electronics, Electrical, Photonics, Physics, Material Science

Theoretical study and modelling of dissipative Kerr solitons in microring resonators

Theme: Communications
Supervisor: Eoin Russell

Background:

Dissipative Kerr solitons (DKSs) are a special waveform that can propagate in optical resonators, resulting in a stable pulse whose shape does not change as it propagates through the cavity. In recent years the phenomenon of soliton formation has been observed in a variety of microring cavities and has seen application in many groundbreaking fields, including optical communication, metrology and spectroscopy [1].

In the time domain, DKSs are described as optical pulses with an unchanging envelope, but their frequency domain behaviour is of particular interest in many applications. In the frequency domain, DKSs produce a spectrum known as an optical frequency comb (OFC) [2]. OFCs are a light spectrum consisting of many discrete wavelengths separated by a near identical frequency spacing. These optical spectra resemble the teeth of a comb, hence the name. OFCs have proven to be incredibly useful in many applications, and their importance was recognized in 2005 with the Nobel prize in physics being awarded to John L. Hall and Theodor W. Hänsch for their contributions to OFC development.

There are many approaches to generate OFCs, but the resulting systems tend to be bulky, expensive and have high power consumption. Using DKS formation in microring resonators to generate OFCs will address the aforementioned issues, resulting in a low-power, cost-effective, chip-scale OFC source. In this project, the aim is to theoretically study the dynamics of DKS and OFC formation in new nonlinear silicon microresonators, predicting the performance of future novel devices.

Methods:

The first stage of the project will consist of studying the literature and fundamental physics of nonlinear optical systems, with a focus on DKSs.

The second stage of the project will involve using a preexisting python code base, called pyLLE, to explore the rich dynamics of soliton formation in microring resonators and make predictions for future experiments.

Predicted results and impact:

The predicted result of this project is a collection of insights into the formation of DKSs and OFCs in silicon based microring resonators. These insights will influence future device designs and potentially open new novel approaches for DKS generation in microring resonators.

References:

1. Tobias J. Kippenberg et al. "Dissipative Kerr solitons in optical microresonators", Science361, eaan8083(2018). DOI:10.1126/science.aan8083.
2. R. Paschotta, article on "Frequency Combs" in the RP Photonics Encyclopedia, retrieved 2024-11-11. https://doi.org/10.61835/h9j
3. Moille, G. , Li, Q. , Lu, X. and Srinivasan, K. (2019), "pyLLE: a Fast and User Friendly Lugiato-Lefever Equation Solver", Journal of Research (NIST JRES), National Institute of Standards and Technology, Gaithersburg, MD. https://doi.org/10.6028/jres.124.012

Location: Tyndall

Type: Fully In-person

Key words: Solitons, Microresonators, Nonlinear Silicon Photonics, Optical Frequency Combs

Degree(s) that will suit this project: Physics, Theoretical Physics, Maths & Physics, Electronic Engineering

Characterization of trench self-patterning in InGaAs/InP: a route to pseudo-substrates for 2 µm applications

Theme: Compound Semiconductors
Supervisor: Emanuele Pelucchi
Co-Supervisor: Camille Barbier

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Background:
III-V semiconductors are key materials for opto-electronic applications due to their broad wavelength tunability. Despite the strong developments in planar devices, the long wavelength range (i.e. > 2 µm) on conventional substrate (InP) is still challenging to reach while keeping good material quality. This complexity arises from the necessity to grow highly lattice-mismatched heterostructures. We recently discovered a new and unexpected physical process: a tensile strain induced trench self-patterning of InGaAs/InP structure which comes at hand to address this challenge. This pseudo-substrate can be exploited to grow strain-balanced quantum wells (SBQWs) emitting at 2 µm, still limiting the defect density.

Methods:
This project will focus on various structural characterization and optimization of the novel InGaAs buffer phenomenology on InP substrates, and the effects on the SBQWs heterostructure. The goal is to reach insights in the unexpected physical processes involved and identify the best growth condition while obviously preserving a good optical emission of the upper SBQW.
Series of InGaAs buffer sample will be grown by MetalOrganic Vapour Phase Epitaxy (MOVPE) with systematic variation of composition and thickness on InP substrate to allow a comprehensive analysis. The initial phase of the project will consist into the characterization of the buffer layers thanks to several experimental techniques. High resolution X-Ray Diffraction (HRXRD) allows to precisely determine the composition and residual strain of the buffer layer. The surface, defects and trenches morphologies will be observed and quantified by Nomarski optical microscope and atomic force microscopy (AFM) with sub nm resolution. The scanning electronic microscopy (SEM) observations correlated with XRD will give us access to the sample thickness, and correlate with the other observations. The second part of the project will address optical properties. Active SBQWs will be grown on the optimized InGaAs buffer layer identified previously. The heterostructures will be (cryogenically) optically characterized by photoluminescence (PL). In a feedback-driven optimization loop, new samples will be grown to improve the QW emission profile.

Predicted results and Impact:

We anticipate that the trench density should increase while the Indium composition is increased as well as the thickness. We expect to observe a trend of the material quality by varying the buffer properties and be able to identify the best growth conditions. This should improve the PL emission of the SBQW heterostructure. The results will provide valuable insights of the relaxation strain mechanism of the trench self-patterning in InGaAs, contributing to the development of long wavelength range device for opto-electronics. Ultimately, this work will serve as the basis for a publication and further collaborative research to implement trench self-patterning buffer as strain management option for several devices.

Location: Tyndall

Type: Fully In-person

Key words: Epitaxy, quantum well, structural characterization, photoluminescence

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

Doping optimization in Nitrogen-polar Gallium Nitride (N-polar GaN)

Theme: Compound Semiconductors
Supervisor: Pietro Pampili

Background:
Gallium Nitride (GaN) is one of the most important semiconductor materials, with many applications in photonics (e.g. blue LEDs and lasers), as well as in RF and power electronics (e.g. high-electron mobility transistors). Our group in Tyndall has a long-standing expertise in epitaxial growth of GaN-based structures using a technique called Metal Organic Vapour Phase Epitaxy (MOVPE).
Due to its unique crystal structure, GaN epitaxy can be done in either one of two distinct directions or polarities: “gallium-polar” or “nitrogen-polar”. Ga-polar MOVPE growth is, by far, the most used approach, because it is easier to control, and usually results in better purity and surface morphology of the materials. N-polar MOVPE growth is much more difficult to control, but has the potential to produce GaN-based structures that are ideally suited to solve some of current limitations of existing GaN devices.
As part of a recent collaboration with Nagoya University, we have developed MOVPE growth techniques to produce high-quality N-polar GaN and other III-Nitride N-polar materials in Tyndall. However, being still a relatively new and not fully understood material, more research and further optimization is still required. This requires extensive structural and electrical characterization of our materials.

Methods:
In particular, the aim of this project is to study the doping of N-polar GaN, which requires different optimization than in standard Ga-polar GaN. The student will have the opportunity to expand their understanding of semiconductor doping, and collaborate to the advancement of a new semiconductor material.
Different sets of samples (both Ga- and N-polar) prepared with varying doping levels and growth conditions will be provided to the student for electrical characterization. The student will learn how to measure free carrier concentration and mobility using various CV and Hall-effect techniques.
The work will consist in sessions of data collection using the equipment available at Tyndall, followed by analysis of the data to extract the main conductivity parameters. The two main objectives of the project are: 1) identify the samples with the highest conductivity to help with the optimization of the growth conditions, and 2) understand what test conditions give reliable results by comparing the different experimental techniques available at Tyndall.

Predicted results and Impact:
Highlight the differences in doping efficiency between Ga- and N-polar GaN.
Opportunities for a paper.

References:

1. M. Pristovsek, I. Furuhashi, and P. Pampili, 'Growth of N-Polar (000-1) GaN in Metal–Organic Vapour Phase Epitaxy on Sapphire', Crystals, vol. 13, no. 7, 2023, doi: 10.3390/cryst13071072.
2. S. Keller et al., 'Recent progress in metal-organic chemical vapor deposition of (000-1) N-polar group-III nitrides', Semicond. Sci. Technol., vol. 29, no. 11, p. 113001, 2014, doi: 10.1088/0268-1242/29/11/113001.
3. N. A. Fichtenbaum et al., 'Electrical characterization of p -type N-polar and Ga-polar GaN grown by metalorganic chemical vapor deposition', Appl. Phys. Lett., vol. 91, no. 17, 2007, doi: 10.1063/1.2800304.

Location: Tyndall

Type: Fully In-person

Key words: Semiconductors, doping, Hall effect measurements

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

Machine-Learning Interatomic Potentials for Alloy Semiconductor Heterostructures

Theme: Compound Semiconductors
Supervisor: Badal Mondal
Co-Supervisor: Stefan Schulz

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Background:
Semiconductor heterostructures with alloyed materials are integral to devices like lasers, transistors, and LEDs. However, alloy disorder and local strain within these structures at atomic scale negatively impact device performance on macroscale by disrupting carrier transport and introducing parasitic pathways.[1] Fully atomistic models are essential for understanding and designing these heterostructures for reliable electronic functionality. While first-principles methods such as density functional theory (DFT) provide high accuracy, they are limited to smaller systems (hundreds to thousands of atoms).
Machine learning (ML) models have demonstrated great success in extending the applicability of atomistic computations, allowing larger systems to be studied accurately and efficiently.[1] This project aims to develop machine-learning interatomic potentials (MLIPs) using the state-of-the-art atomic cluster expansion (ACE) ML model [2] to accelerate atomistic computations. We will apply this framework to Silicon-Germanium (Si-Ge) alloy heterostructures, which are widely used in electronics, optoelectronics, and quantum computing.[1] The ACE model has demonstrated remarkable data and computational efficiency, enabling scalable performance as system size increases.[3] Unlike prior methods [1] that rely on additional feature engineering (e.g., Voronoi tessellation), the ACE model inherently provides a complete descriptor of the local atomic environment, directly capturing local strain fields and their effects. This streamlined approach will enable accurate large-scale modelling by linking DFT and ML simulations, enhancing computational design capabilities for advanced devices.

Methods:
1. DFT Calculations: We will begin by performing DFT calculations on various Si-Ge superlattice (SL) configurations. We will conduct the DFT calculations on high-performance clusters using the Vienna Ab initio Simulation Package (VASP) software.[4a] First, we will create multiple Si_nGe_m SL units by stacking layers along the [001] direction, where n and m represent the number of Si and Ge monolayers in each unit cell. In these ordered structures, Si and Ge layers are arranged in a regular pattern. To create disordered structures, we will randomly replace some Si atoms with Ge atoms to produce different compositions. These structures will serve as the data set for training our ML model in the next step.

2. Training the ACE ML Model: Next, we will train an ACE model to construct interatomic potentials based on the DFT reference data obtained in step-1, using the ACEpotentials.jl, a Julia-language software package.[4b] We will also write (basic level) Julia code to run this package and perform post-processing tasks. We will use a part of the DFT data from step-1 to train the ACE model for MLIP, while the remaining data will be used to test the ML model's performance. Finally, we will benchmark our developed ACE model against previous ML models from Ref. [1], particularly in training time and accuracy.

Predicted results and Impact:

- Gain hands-on experience with modern atomistic simulation tools, including pre- and post-processing techniques.
- Develop skills in performing advanced DFT calculations on high-performance clusters.
- Build expertise in training ML models within a simulation framework.
- Opportunities for contributions to research publications.

References:

[1] Pimachev, A.K., and Neogi, S. "First-principles prediction of electronic transport in fabricated semiconductor heterostructures via physics-aware machine learning." npj Comput Mater 7, 93 (2021). doi: https://doi.org/10.1038/s41524-021-00562-0
[2] Drautz, R. "Atomic cluster expansion for accurate and transferable interatomic potentials." Phys. Rev. B Condens. Matter. 99, 014104 (2019). doi: https://doi.org/10.1103/PhysRevB.99.014104
[3] W. C. Witt, C. van der Oord, E. Gelžinyté, T. Järvinen, A. Ross, J. P. Darby, C. H. Ho, W. J. Baldwin, M. Sachs, J. Kermode, N. Bernstein, G. Csányi, and C. Ortner. "ACEpotentials.jl: A Julia implementation of the atomic cluster expansion." J. Chem. Phys. 159, 164101 (2023). doi: https://doi.org/10.1063/5.0158783
[4a] "Vienna Ab initio Simulation Package", https://www.vasp.at (last accessed 10.11.2024).
[4b] "ACEpotentials.jl Documentation", https://acesuit.github.io/ACEpotentials.jl/stable (last accessed 10.11.2024).

Location: Tyndall **Type**: Fully In-person

Key words: simulations, modelling,density-functional-theory, machine-learning

Degree(s) that will suit this project: Physics, Computer science, Mathematics, Chemistry

Detection of microplastics in water samples using electrochemical sensor

Theme: Environment & Energy
Supervisor: Tarun Narayan
Co-Supervisor: Alan O'Riordan

Tyndall National Institute
Institiúid Náisiúnta

Background:
Microplastics—tiny plastic particles less than 5 mm in size—have become pervasive in the environment, found in oceans, rivers, soils, and even in the air. These particles originate from larger plastic debris breaking down or from direct sources like microbeads in cosmetics and fibers from synthetic clothing. On average, humans consume between 0.1 to 5 grams of microplastics per week, equivalent to approximately 5 grams per month, or about 250 grams per year. This is comparable to the weight of a credit card each week. Microplastics enter the human body mainly through contaminated food, water, and even air. Studies link microplastic exposure to potential toxic effects, as these particles can carry harmful chemicals, disrupt ecosystems, and accumulate in organisms. Addressing microplastic pollution is critical to safeguarding biodiversity, food safety, and public health, driving the urgent need for effective monitoring, management, and reduction strategies.

Methods:
Electrochemical sensors leverage the unique electrical and chemical properties of microplastics, such as surface charge and hydrophobicity, allowing for real-time, on-site analysis. These sensors utilize diverse materials like carbon nanomaterials, metal nanoparticles, and conductive polymers as active sensing elements to enhance sensitivity and signal stability. Recent advances focus on improving sensor specificity for different microplastic types, enhancing signal transduction mechanisms, and integrating data processing capabilities for portable applications. This project will focus on the principles, design, and performance of microplastic electrochemical sensors, along with challenges like sensor fouling, selectivity limitations, and environmental variability.

Predicted results and impact:
Predicted outcomes include the ability to detect trace levels of microplastics in complex environmental samples like ocean water, soil, and air with minimal preparation. These sensors are anticipated to offer selective detection, differentiating types of microplastics based on particle size, shape, or polymer type, enhancing both research and regulatory efforts. Real-time data from electrochemical sensors would allow for quick responses to microplastic pollution events, enabling better regulation and pollution control, particularly in high-risk areas like water bodies and agricultural soils.

References:

A Practical Beginner's Guide to Cyclic Voltammetry | Journal of Chemical Education (acs.org)

Location: Tyndall

Type: Fully in-person

Key words: electrochemistry, material science, environmental monitoring

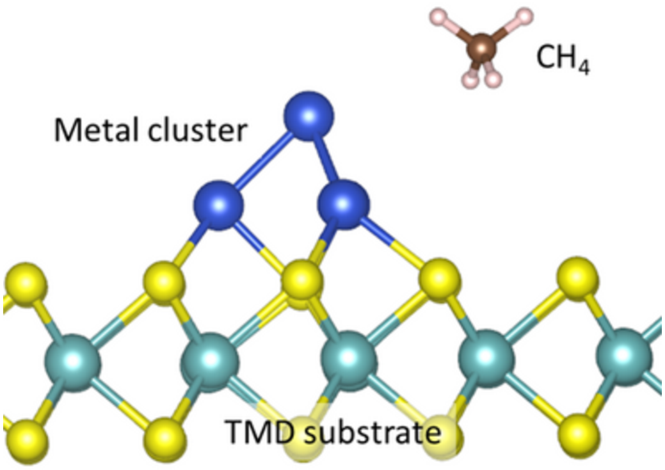
Degree(s) that will suit this project: Chemistry, industrial chemistry, materials engineering, Bio-chemistry

Machine-learning assisted modelling of methane activation on 2D materials

Theme: Environment & Energy
Supervisor: Cara-Lena Nies

IPIC
BRINGING PHOTONICS TO LIFE

Background:
The air pollutant methane (CH_4), produced mainly through agriculture, industry, and fossil fuel-based energy production, poses an escalating threat to the environment. Catalysis presents the critical pathway to resolving this threat, while also providing a sustainable route towards production of methanol and other platform chemicals through direct, partial CH_4 oxidation. However, existing methane oxidation catalysts are inadequate – they use rare and expensive materials (e.g., Pt, Pd Au/C, RuO2[1]), provide no high-yield routes to high-value products, and/or have poor selectivity, producing only CO_2 rather than the partial oxidation products which provide a valuable, renewable route to molecules essential to energy storage and industrial chemistry applications. The first critical step in converting CH_4 is the breaking of the C-H bond. The energy required to achieve this in the gas phase is only overcome at very high process temperatures. With a catalyst, the required energy input can be significantly reduced, however the specific activation energy is affected by the catalyst materials, surface facets, as well as metal nanoparticles loaded onto the surface. Therefore, when designing a catalyst for CH_4 oxidation it is crucial to first optimise the activation energy at this initial activation step.
Layered materials, such as graphene and transition metal dichalcogenides (TMDs), can be exfoliated into individual, ultrathin 2D monolayers and are of interest for a wide variety of materials applications due to their varied properties. Ultrathin catalysts made from 2D materials have many advantages including a large surface to volume ratio, which provides a large number of active sites. 2D monolayers decorated with small metal clusters provide a route toward catalysts, which use either less of the rare and expensive materials currently in use or an alternative material.
This project will investigate the activation of CH_4 using small Cu, Co and Ru clusters on 2D TMDs (MoS_2, WS_2, WSe_2) to explore their use as CH conversion catalysis.



Methods:

To model the activation of CH_4[1] on TMD surfaces[2], we will use a combination of atomic-scale simulation tools, namely density functional theory (DFT) and a machine learning (ML) potential created using DFT data and the DeePMD tool kit[3]. DFT is a state-of-the-art, quantum mechanical approach to study materials and their properties; in this case, we will use it to study the interactions between CH_4 and small metal clusters adsorbed on TMD monolayers. Calculating the activation energy for breaking the C-H bond is extremely resource intensive using DFT and we will therefore use the ML potential to obtain this important performance metric at a reduced computational cost.

Predicted results and impact:

The scientific aim of this project is to explore TMDs as potential CH_4 conversion catalysts and understand how metal clusters and TMD substrate can affect the activation energy required to break the C-H bond. The student working on this project will (i) learn to use state-of-the-art DFT and ML tools and (ii) gain experience in using materials modelling to study important material properties, such as activation energies.

References:

1. J. J. Carey and M. Nolan, Applied Catalysis B: Environmental (2016), 197, 324–336. https://doi.org/10.1016/j.apcatb.2016.04.004
2. C.-L. Nies and M. Nolan, Beilstein J. Nanotechnol. (2021), 12, 704–724. https://doi.org/10.3762/bjnano.12.56
3. https://deepmodeling.com/space/DeePMD-kit

Location: Tyndall

Type: Hybrid, min 3 days in person

Key words: materials modelling, methane conversion, 2D materials, density functional theory, machine learning

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

Ultra-low Power (ULP), Energy-Harvesting (EH) PMIC & Wireless Power Transfer (WPT) for implantable devices

MCCI
SOLVE THE IMPOSSIBLE

Theme: Environment & Energy
Supervisor: Hugo Cruz

Background:
Envisage a programmable ULP-EH Power Management SoC (ULP EH PMSoC) platform which has all necessary blocks to implement AC-DC or DC-DC converters for ultra-low power ambient energy harvesting applications, with various sources, such as DC - PV, TEG or AC – Vibrational (PZT or EM). This ULP Power Path utilizes MAGoS and MAGiP inductor devices fabricated by Tyndall FAMES Magnetic Pilot-line. For the building blocks we project a fully digital and flexible configurable platform with ULP Control [1][2] and with the aim to further reduce state-of-the-art cold start voltages to ~10mV – AC or DC. There are many blocks of circuit overlap between the requirements of WPT and ULP – in terms of active rectifiers, integrated magnetic inductive couplers and ULP controller circuits.

Methods:
The project aims at computer simulations in Cadence and possible tape-out using XFAB 0.18um SOI; depending on the student progress. Several blocks will be ready, and the student will be able to do system simulations, or single block design. The blocks available will be:
The available building blocks which require circuit simulation and possible improvement using the Cadence platform are

1. Ultra-low-power SAR ADC
2. Digital Compensation for the DC-DC converter
3. Frequency modulator for DC-DC buck converter.
4. Analog power path (DC-DC buck converter)
5. Wireless power transfer active rectifier.

Cold start circuit architecture

Predicted results and impact:
We offer an opportunity to work on a state-of-the-art flexible, programable Power Management Integrated Circuit (ULP EH PMSoC) architectures that are capable of handling different low-power energy-harvesting (EH) sources, various energy storage types and cater for a wide spectrum of variable, intermittent loads, including RF transceiver loads, high accuracy sensors, and photonics applications.
Aim to reduce by half the cold-start voltage of current state-of-the-art publications for Energy Harvesting.

We have already a large base of innovations to build on: World’s first MAGoS 1:11 turns ratio cold start Tx and 15 MHz cold start circuits.
Our Cold Start Tx is 1,000 times smaller. Innovative DTC with bank of 7 oscillators and all digital PLL to offer ULP unified time-base over nano seconds to hours!

References:

1. W. Peng, X. Yue, L. Pakula and S. Du, "A Capacitor-Based Bias-Flip Rectifier with Electrostatic Charge Boosting for Triboelectric Energy Harvesting Achieving Auto-MPPT at Breakdown Voltage and 14× Power Extraction Improvement," 2024 IEEE International Solid-State Circuits Conference (ISSCC), San Francisco, CA, USA, 2024, pp. 516-518.
2. X. Yue, S. Javvaji, Z. Tang, K. A. A. Makinwa and S. Du, "A Bias-Flip Rectifier with a Duty-Cycle-Based MPPT Algorithm for Piezoelectric Energy Harvesting with 98% Peak MPPT Efficiency and 738% Energy-Extraction Enhancement," 2023 IEEE International Solid-State Circuits Conference (ISSCC), San Francisco, CA, USA, 2023, pp. 442-444.

Location: Tyndall

Type: Fully in-person

Key words: Ultra-low Power, ULP, Energy-Harvesting (EH) PMIC & Wireless Power Transfer (WPT)

Degree(s) that will suit this project: Electrical/Electronics engineering

Fluorescence lifetime imaging for diagnostics of inflammatory bowel diseases.

Theme: Health & Wellbeing
Supervisor: Katarzyna Komolibus
Co-Supervisor: Sanathana Konugolu Venkata Sekar, Sumedha Chanda

IPIC
BRINGING PHOTONICS TO LIFE

Background:
In the past decade, Inflammatory Bowel Disease (IBD) has emerged as a public health challenge worldwide. IBD, namely Crohn's disease (CD) and ulcerative colitis (UC), can affect any segment of the gastrointestinal (GI) tract carrying significant morbidity and mortality. Projections indicate that by 2030, the Western world may experience alarming surge in IBD cases with estimated number of affected people over 10 million. Unfortunately, IBD is challenging to diagnose as it develops progressively over several years and presents with set of clinical symptoms that are often vague and overlap with other GI diseases. Endoscopic imaging has gained traction as an in situ method to visualize inflammation and is instrumental to diagnosing IBD and its subtypes. However, most imaging approaches lack sensitivity to early inflammatory events and require additional contrast agents. New strategies to directly detect early signs of inflammation would improve patient's prognosis and alleviate the health care associated costs of disease management.

Methods:
Autofluorescence imaging is a simple technique based on emission from tissue's endogenous fluorophores (e.g. collagen, NADH), which has shown promise to detect inflammation in IBD-associated patients. On the other hand, fluorescence lifetime imaging (FLIm) is sensitive to the tissue microenvironment, and thus it adds a new dimension to characterize the lesions. Compared to intensity measurements, lifetime is a more robust metric because it is less sensitive to artifacts created by imaging parameters such as variations in probe-to-tissue distance. The project will be part of extension of ongoing clinical study on IBD and it will involve (1) hands-on experimental system characterisation and optimisation using fluorescence lifetime phantoms, (2) measurements of tissue sections using FLIm microscope, (3) image and data analysis.

Predicted results and impact:
The project's aim will be to identify optimised spectral bands for the detection of IBD and designing the optimised system layout according to preliminary results. Intern will get hands-on experience with building experimental setups, data acquisition, algorithm development and processing.

References:

1. Alfonso-Garcia A., Cevallos S.A., Lee J.-Y., Li C., Bec J., Bäumler A.J., Marcu L., Assessment of Murine Colon Inflammation Using Intraluminal Fluorescence Lifetime Imaging, Molecules 27, 1317 (2022) https://doi.org/10.3390/molecules27041317
2. Coda S., Thompson A.J., Kennedy G.T., Roche K.L., Ayaru L., Bansi D.S., Stamp G.W., Thillainayagam A.V. , French P.M.W., Dunsby C., Fluorescence lifetime spectroscopy of tissue autofluorescence in normal and diseased colon measured ex vivo using a fiber-optic probe, Biomed. Opt. Express 5, 515-538 (2014) https://doi.org/10.1364/BOE.5.000515

Location: Tyndall

Type: Fully in-person

Key words: biophotonics, fluorescence lifetime imaging, optics, data analysis

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

Handheld High-Performance Time of Flight System to develop Integrated Fast Accurate Scalable Technologies (FAST) for biophotonics applications.

Theme: Health & Wellbeing
Supervisor: Suraj Kumar Kothuri
Co-Supervisor: Sanathana Konugolu Venkata Sekar, Pranav Lanka

IPIC BRINGING PHOTONICS TO LIFE

Background:
Over the past three decades, advancements in the photonics industry have enabled scientists to leverage light for understanding complex biological processes within the body. This progress has led to the development of a wide array of innovative devices that use light as a non-invasive means to probe physiological functions. Recent breakthroughs in semiconductor technology, combined with biophotonics and improved data analysis methods, have further paved the way for miniaturized, accurate, and safe diagnostic tools. Most of them are now available in wearable formats. Today, physiological metrics such as heart rate, respiration, sleep patterns, ECG, blood oxygen saturation, and menstrual cycles can be monitored conveniently from a wrist-worn device.
However, current technology faces limitations, particularly in its ability to penetrate deeper regions of the body. To address this, photon Time-of-Flight (pToF) spectroscopy emerges as a promising alternative to existing Continuous Wave (CW) methods. pToF offers significant advantages in overcoming practical challenges like skin pigmentation variability, motion artifacts, and low blood perfusion conditions, enhancing the accuracy and reliability of future era of biophotonic diagnostics.
In this project, the intern will actively participate in ongoing research and development efforts at our Integrated Fast Accurate Scalable Technologies (Integrated FAST) wing of Biophotonics@tyndall group, contributing to innovations aimed at refining and expanding wearable biophotonic applications. In particular, the intern will be invested in handheld high-performance Time of Flight system (similar to LiDAR) for biophotonics.

Methods:
Experimental Activities:
Characterizing the well-established MEDPHOT 16 tissue mimicking phantom kit to assess the system's accuracy, stability & reproducibility followed by extraction of the optical properties of the same.
Hands-on involvement in the development of optical system for performing in vivo studies on human volunteers.

Theoretical activities:
The data analysis of the pToF curves is performed using diffusion models based on analytical or Monte-Carlo solutions. The intern will be given training on the instrument building aspects of photon Time-of-Flight system with a systematic procedure to characterize and validate a given biophotonics system. Data analysis to extract optical properties of the biological media. Data analysis of spectroscopic data obtained from in vivo human studies.

Predicted results and impact:
Project Aims - Using flexible, transparent, and affordable PDMS, we aim to optimise a small-scale spectroscopic device, integrating a portable optical fiber for convenient monitoring.[4, 5]

References:

1. Li et al., Journal of Biomedical Materials Research Part A, 2013.
2. Dorozhkin, Biomaterials, 2010.
3. Raynaud et al., Biomaterials, 2002.
4. McDonald & Whitesides, Accounts of Chemical Research, 2002.
5. Lee et al., Biosensors and Bioelectronics, 2011.

Location: Tyndall

Type: Fully in-person

Key words: Hydrogels, Medical Devices, Spectroscopy, Data Analysis, Cell Culture

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

Long-wavelength Near infrAred optical Signals for Continuous non-invasivE Nascent life well-being monitoring

Theme: Health & Wellbeing
Supervisor: Shree Krishnamoorthy
Co-Supervisor: Rekha Gautam

Background:
Nascent life, the period just before birth, during labour, and through the first week of life, remains the most precarious [1]. Two in every thousand babies suffer after-effects of pre-term hypoxia and die. Better monitoring methods are needed to improve healthcare for these babies [2]. NASCENT will develop a novel spectroscopic pH measurement, a gold standard for hypoxic distress.

Methods:
RF-modulated lasers will be used to probe the water absorption bands around 1480 and 1900 nm in water phantoms of 0.5 mm thickness [3]. The work involves aspects of signal processing, lasers and photonics detection schemes. Different of this project suits those interested in experiments, numerical or theoretical work in optical communications.

Predicted results and impact:
A proof-of-principle for a novel spectroscopy scheme will be tested in this internship either through numerical modelling, electrical circuit analogue build or theory development depending on students strengths. This will be a stepping stone to developing a full novel spectroscopy technique.

References:
[1] Malin, Gemma L., Rachel K. Morris, and Khalid S. Khan. "Strength of association between umbilical cord pH and perinatal and long-term outcomes: systematic review and meta-analysis." BMJ 340 (2010).
[2] Cummins, Gerard, et al. "Sensors for fetal hypoxia and metabolic acidosis: a review." Sensors 18.8 (2018): 2648.
[3] S. Krishnamoorthy, et al. "Non-invasive continuous hypoxia assessment in intra-partum fetus through long wavelength near infrared spectroscopy." Photonic Instrumentation Engineering X. Vol. 12428. SPIE, 2023.

Location: Tyndall **Type**: Fully in-person

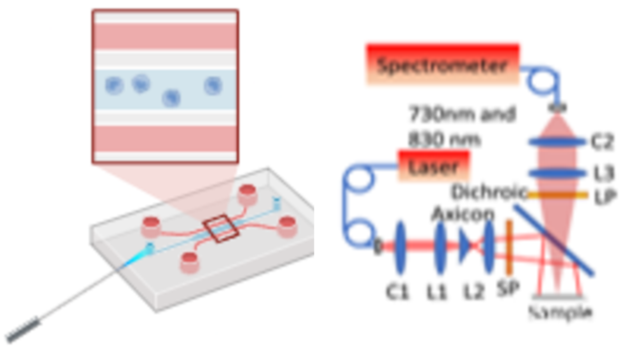
Key words: laser spectroscopy, molecular spectroscopy, optical spectroscopy, dispersion, near-infrared spectroscopy, Refractive Index Change, BioPhotonics, vibrational spectroscopy

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

Optimisation of a Hydrogel-Based Miniaturised Platform for nHA Detection

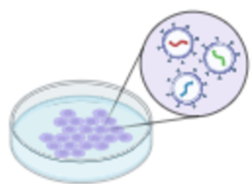
Theme: Health & Wellbeing
Supervisor: Imanda Jayawardena

Background:
Nano-hydroxyapatite (nHA) plays a vital role in biomedical applications due to its biocompatibility and osteoconductive properties. It is used in bone tissue engineering, dental applications, and as a drug delivery carrier[1,2] .Utilising a miniaturised platform for nHA detection offers portability, cost-efficiency, and the potential for point-of-care diagnostics[3], beneficial for in-situ analysis during surgeries or post-implant monitoring. Polydimethylsiloxane (PDMS), used in the fabrication of miniaturised platforms is flexible, biocompatible, optically transparent, and relatively inexpensive, making it ideal for developing small-scale devices for biomedical diagnostics[4]. Its transparency allows effective light transmission in spectroscopic techniques. Optical fibers can deliver and collect light signals efficiently, making them suitable for remote or flexible monitoring of nHA5. Thus, integration of an optical probe enables more versatile, flexible spectroscopic analysis in clinical or biomedical environments, ensuring that the miniaturised device remains highly functional and adaptable to various settings.



Methods:
Research Activities
Below are research activities that you would be expected to undertake during this project. Further information, resources and training would be provided to the successful candidate.

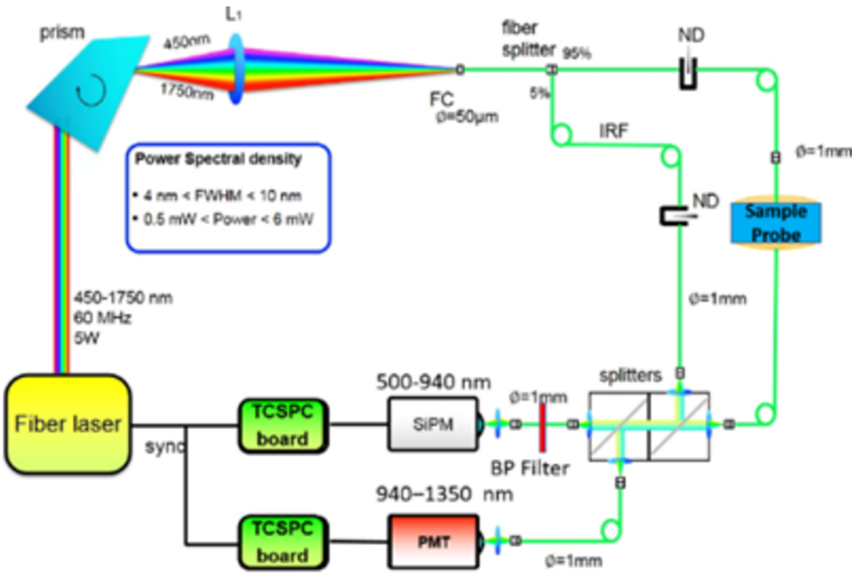
- Optimise the miniaturised PDMS device
- Prepare hydrogel-nHA samples of varying compositions within the device
- Acquire Raman spectra of hydrogel-nHA samples
- Assemble an optical probe using optical fibers and integrate it into the device
- Data analysis and interpretation
- Optional/Time-Permitting Research Activities
- Cell culture studies on the hydrogel substrates within the optimised device



Predicted results and impact:
Intern will have exposure to both experimental and theoretical work. The activity is aligned with the labs goal to build next generation wearable device for fitness and biomedical parameter monitoring applications, so intern will directly participate in the development of breakthrough technologies.

References:

1. Konugolu Venkata Sekar, S.; Lanka, P.; Farina, A.; Dalla Mora, A.; Andersson-Engels, S.; Taroni, P.; Pifferi, A. Broadband Time Domain Diffuse Optical Reflectance Spectroscopy: A Review of Systems, Methods, and Applications. Appl. Sci. 2019, 9, 5465. https://doi.org/10.3390/app9245465



Location: Tyndall

Type: Fully in-person

Key words: Time-of-flight, biophotonics, computation models, Matlab, simulations, python, optics, instrumentation.

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

Reliability study of PZT for application in medical implant

Theme: Health & Wellbeing
Supervisor: Ruth Houlihan

Background:
Micropump-based devices currently under development at Boston Scientific are driven by piezoelectric materials – those that can generate an electrical charge in response to an applied mechanical stress, or conversely, generate a mechanical strain in response to an applied electric field. This property arises from the asymmetric arrangement of atoms or molecules in the crystal lattice of the material, which causes a displacement of charges when the material is deformed. In order to fully understand the characteristics of these materials, and their impact on pump performance, significant amounts of data relating to the physical characteristics of piezoelectric materials needs to be acquired and processed.
Medical implants employing PZT actuators are being designed and fabricated by Boston Scientific. These implants will be required to operate reliably in the body for 10 years. Extensive testing of the PZT component in this assembly is necessary to understand potential failure mechanisms and to predict lifetime. Testing will include electrical and mechanical tests and will primarily focus on lifetime reliability and failure analysis. To this end, this project will use our state-of-the-art experiment characterisation infrastructure in Tyndall.

Methods:
Electrical Testing: Electrical testing will include impedance measurements and leakage current measurements. The student will be trained in the use of parameter analyser and LCR meter.
Electro-Mechanical Testing: Characterisation of the piezo-electric properties of the PZT material using a piezo-meter. Laser Doppler Vibrometry (LDV) may also be used for analysing component performance and mechanical resonance.

Reliability Test Development: Reliability and lifetime test development specific to the component. This will require a fundamental understanding of the physical degradation mechanisms specific to multi-layer PZT actuators in the context of a medical implant application. Ultimately the designed test will be a dedicated acceleration test to predict lifetime for soft PZT actuators.

Predicted results and impact:

The output of this work is towards a product currently in development by Boston Scientific and which is being led by a team in Clonmel. The PZT actuator is a critical component of this product which must maintain performance and reliability over at least 10 years. This PZT actuator is currently acquired by Boston from external suppliers and so they have limited control over product quality. Screening incoming material will be essential therefore in product development.

The objective of this project is to help understand degradation mechanisms in the materials through extensive failure analysis (FA). The FA work will be achieved through electrical, piezoelectric and electro-mechanical testing.

References:

1. https://www.bostonscientific.com/
2. P. Pertsch, S. Richter, D. Kopsch, N. Krämer, J. Pogodzik, E. Hennig, Reliability of Piezoelectric Multilayer Actuators, ACTUATOR conference, Bremen, Germany, June 14 – 16, 2006

Location: Tyndall

Type: Fully in-person

Key words: reliability, PZT, piezoelectric, micro-pump

Degree(s) that will suit this project: Mechanical engineering, electrical engineering, physics

Quantum light emitters: Tailoring the optical properties of quantum dots with magnetic fields

Theme: Quantum
Supervisor: Stefan Schulz
Co-Supervisor: Neil O'Connor

Background:
One of the most critical challenges in advancing quantum information processing (QIP) and quantum computing is scaling current laboratory systems to larger numbers of qubits. To address this challenge, so-called multi-dimensional photonic cluster states have been proposed as an ideal solution [1] when used as the substrate for quantum computation. Semiconductor quantum dots (QDs), which are often described as artificial atoms, are promising sources for generating these highly entangled quantum states. However, current realisations predominantly rely on probabilistic fusion gates, rather than direct generation of cluster states [2].

This project focuses understanding the electronic structure of site-controlled QDs grown at Tyndall, which exhibit high controllability of the structural properties of these dots, e.g. size and shape [3]. These features make them ideal candidates for deterministic direct generation of multi-dimensional photonic cluster states, thus eliminating the need for probabilistic fusion gates. On one hand side, electronic structure needs to be understood. This includes the energetic separation of energy levels in such an artificial atom as well as understanding the symmetry of the involved states (s-like or px-likestates as in an hydrogen atom). Moreover, to tailor and ultimately realise photonic cluster states, the QDs have to be exposed to (strong) magnetic fields. This latter aspect presents an additional challenge for the theoretical modelling and thus for guiding the design of QD based photonic cluster state emitters.

Methods:
The aim of this project is (i) to develop a theoretical model that accounts for magnetic fields in the Schrödinger equation to describe the electronic structure of semiconductor QDs and (ii) to analyse the influence of magnetic field on the electronic and ultimately optical properties of semiconductor QDs grown in Tyndall. The project will start with simpler (one- or two dimensional) simulations using for instance the finite difference method (FDM) to solve the Schrödinger equation to gain initial insights into the electronic structure of (i) artificial atoms and (ii) modifications induced by magnetic fields.

As the project progresses, we aim expand the model to a full three-dimensional simulation of QD structures targeted experimentally in Tyndall using models available in the group. This approach will allow for a more accurate and detailed representation of the system, providing critical insights into the electronic and optical properties of the QDs ideally allowing for comparison with experimental data.

Predicted results and impact:
By the end of the project, the developed model shall elucidate the impact of magnetic fields on the electronic structure of site-controlled QDs experimentally realised in Tyndall. Overall, the theoretical results shall provide essential contributions for the ongoing work at Tyndall and shall help in aiding the experimental realization of multi-dimensional cluster states using QDs. Furthermore, this theoretical foundation can support other researchers investigating similar QD systems or working towards deterministic quantum light sources, potentially influencing the broader field of quantum optics.

References:

1. S. Economou et al., PRL 105, 093601 (2010).
2. D. Cogan et al., Nat. Photon. 17, 324–329 (2023).
3. L. O. Mereni et al., Appl. Phys. Lett. 94, 223121 (2009).

Location: Tyndall

Type: Fully in-person

Key words: Schrödinger equation, magnetic field, finite-difference method, k.p theory, photonic cluster states, quantum dots

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

Theory of semiconductor quantum wells as tunable quantum materials

Theme: Quantum
Supervisor: Christopher Broderick

Background:
A quantum well (QW) is a "heterostructure" formed by sandwiching a thin layer of a narrow band gap semiconductor ("well") between two layers of a wider band gap semiconductor ("barriers"). Varying the material composition and thickness of the well/barrier layers renders QW electronic properties highly tunable. QWs are ubiquitous in photonics, where they form the active region of devices including lasers and amplifiers. For certain choices of materials and layer thicknesses the QW band gap can be closed, generating an "inverted" band gap [1]. This inverted band gap can produce a "topological insulator" – i.e. a material that conducts electricity around its edge, but remains insulating in its bulk. That the QW can remain insulating in its bulk results from the opening of a band gap via the spin-orbit interaction (SOI). For practical applications it is desirable that this bulk band gap be large vs. the thermal energy k_BT [2].

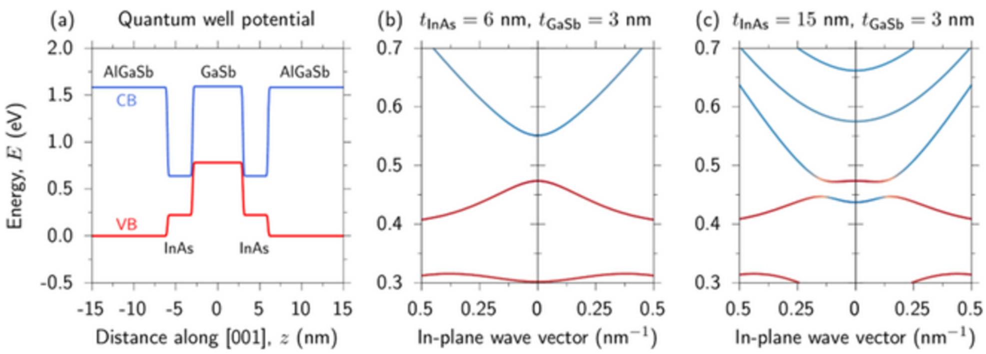


Figure 1. (a) Potential profile of an InAs/GaSb QW. Depending on the layer thicknesses the QW has (b) a conventional band gap, or (c) an inverted band gap, with a small band gap opening via the SOI.

Methods:
This theoretical/computational project will be exploratory in nature. You will learn to simulate the electronic structure of semiconductor QWs and, by analysing QW wave functions, establish what can be ascertained about their properties as tunable quantum materials. You will apply our in-house code [3] to solve Schrödinger's equation for QWs and then, using the QW wave functions, you will write code to calculate technologically-relevant quantum properties (e.g., one property of interest is the spin expectation value and its dependence on wave vector **k**).

Predicted results and impact:
Growth of semiconductor QWs, and fabrication of QW-based devices, is well established and highly advanced in academia and industry. This makes QWs an appealing platform to realise future quantum technologies. The expected outcome of this project is to guide growth and experiment by quantifying the ability to tune the quantum properties of realistic QWs by (i) identifying promising combinations of QW materials and layer thicknesses, and (ii) tuning the quantum properties via an applied electric field.

References:

1. Sci. Adv. 4, eaap7529 (2018)
2. Phys. Rev. Research 4, L042042 (2022)
3. J. Phys. D: Appl. Phys. 57, 035103 (2024)

Location: Tyndall

Type: Fully in-person

Key words: Semiconductors, quantum materials, condensed matter theory, computational physics

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

Data Communication with Visible Light Emitting Diodes

Theme: Wafer Scale & Chip Technologies
Supervisor: Zhi Li

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): https://onlinelibrary.wiley.com/doi/10.1002/adpr.202100312
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: Fully in-person

Key words: LEDs, VLC, and communication

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

Frequency Control of Microwave Photonic Integrated Circuits

Theme: Wafer Scale & Chip Technologies
Supervisor: Fatih Atar

Background:
Use of photonic systems to replace, complement or out-perform the functionalities of microwave electronic devices has been called "Microwave Photonics". Such photonic systems used to be limited to expensive and bulky setups. Utilization of photonic integrated circuits (PICs - small chips on which light can travel, carrying "information") has the promise to miniaturize these systems to the chip scale. Development of photonic devices (lasers, modulators, and photodetectors) for integration on such photonic chips is a very active field of study at Tyndall National Institute and has constantly opened up new research challenges.
One of the challenges associated with this approach is to obtain stable, single-frequency emission from the on-chip lasers. Different photonic devices has been proposed towards this goal but a chip that is capable of self-monitoring its lasing wavelength and fine tuning it to the set value is highly desired for some applications.

Methods:
Photonic integrated circuit (PIC) design, photonic device characterization, high frequency electronic device characterization

Predicted results and impact:
The goal of this project will be to design PICs that are capable of monitoring and stabilizing the operation wavelength of the lasers integrated on the chip. The student will learn characterization of the PIC and various photonic devices, carry out simulation/modelling of PICs on Lumerical (Interconnect) software and design PICs that can achieve the said wavelength monitoring/stabilization functionality. The student will use existing PICs for the initial characterization and will prove the feasibility of her/his proposed approach with modelling and simulations. Potentially the designed circuit (sub-circuit) will be used in many of our future PIC designs, get fabricated at Tyndall and tested for future utilization and publications.

References:

1. MARPAUNG, David, et al., Integrated microwave photonics, Nature photonics, 2019, 13.2: 80-90.
2. KOBAYASHI, Naoki, et al. Silicon photonic hybrid ring-filter external cavity wavelength tunable lasers. Journal of Lightwave Technology, 2015, 33.6: 1241-1246.
3. KOMLJENOVIC, Tin, et al. Widely tunable narrow-linewidth monolithically integrated external-cavity semiconductor lasers. IEEE Journal of Selected Topics in Quantum Electronics, 2015, 21.6: 214-222.
4. Atar, Fatih Bilge, et al. "On-Chip Microwave Photonic System Through Multi-Component Micro-Transfer Print Integration." 2024 International Topical Meeting on Microwave Photonics (MWP). IEEE, 2024.

Location: Tyndall

Type: Fully in-person

Key words: Integrated photonics, microwave photonics, heterogeneous integration

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

Laser power conversion

Theme: Wafer Scale & Chip Technologies
Supervisor: Brian Corbett

Background:
Light from the sun powers the earth directly through photovoltaics, the winds and photosynthesis. Lasers carry optical power that also can be converted to electric power using a photovoltaic cell. High conversion efficiency can be expected since the wavelength is narrowband and thus the optimum bandgap of the photovoltaic device can be selected. As a result power can be transmitted over free space to difficult-to-reach locations where voltage isolation is imperative, or via optical fibres where electrical power is either forbidden.

Methods:
The key steps to optimising the performance of a power converter are the choices of an efficient laser and cell together with the coupling of the light. The student will study the photovoltaic properties of semiconductor devices and the connection to lasers. Power conversion will be investigated experimentally consists of coupling a high power laser to a cell based on a light emitting diode and measuring the resultant current-voltage characteristics as a function of input power and wavelength. The data will be analysed to lead to improved performance through better light distribution and better device selection.

Predicted results and impact:
Power conversion of the incident light to electrical power of > 50%. Better understanding of the factors involved and defining a roadmap to > 60% power conversion. The results will help the uptake of laser power conversion in new applications such as powering devices during surgery and in powering the next upcoming terminals for 5/6G communication terminals, for example.

References:

1. C. Algora, et al, Beaming power: Photovoltaic laser power converters for power-by-light. Joule 6, 340 (2022). https://doi.org/10.1016/j.joule.2021.11.014.
2. P Doguet, et al, An optoelectronic implantable neurostimulation platform allowing full MRI safety and optical sensing and communication, Scientific reports 14 11110 (2024) https://www.nature.com/articles/s41598-024-61330-w
3. B Roycroft, et al., Laser to laser power conversion with remote signalling, Optics Express 29, 16611 (2021). https://opg.optica.org/oe/fulltext.cfm?uri=oe-29-11-16611

Location: Tyndall

Type: Fully in-person

Key words: Power, Lasers, Photovoltaics, Fibres

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

Lasers and photonic devices: characterisation and design

Theme: Wafer Scale & Chip Technologies
Supervisor: Frank Peters

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Background:
Semiconductor lasers and other photonics devices are part of our daily lives, as they are a key element in areas as diverse as internet communications, computer mice, and optical storage (e.g. DVD readers). But, the actual operation of a laser or optical modulator is much more interesting, as semiconductor lasers are nonlinear optical noise amplifiers based on optical waveguides, while optical modulators require quantum engineering and design. The operation of these photonics devices and the propagation of laser emission in a photonic integrated circuit can be explored using various computer-based models.
Once designed, photonic devices are fabricated in a clean room, where the semiconductor is processed using various techniques, such as wet and dry etching, metal and dielectric deposition, and the use of optical masks with photoresist. Once complete, the devices are characterised in test labs, where the optical and electrical properties are evaluated.

Methods:
This internship is designed to be a lab-based project, where characterisation of photonic devices are made using LabVIEW (possibly Python). This will enable the student an opportunity to work on real devices, so they can better understand of the physics. In addition, the theoretical aspects of the lasers can be studied as this will lead to better understanding of the experiments. [1-2] The focus of this internship is the characterisation of coupled lasers built into photonic integrated circuits (PICs). Historically, we have looked at where these coupled laser systems are stable, however for this project the goal will be to investigate areas of instability, including where the coupled lasers show dynamic behaviour such as pulsations.
There is a optional theoretical extension to this project, where the summer intern would learn to simulate these coupled laser systems. This can be useful and instructive to understand the discovered behaviour.

Predicted results and impact:
The intern will learn how to characterise die based lasers and photonics integrated circuits (PICs). Through automated testing multiple different types of laser dynamics will be encountered. This identification will be used to better understand coupled laser systems, which have useful applications in communication and quantum computation.

References:

1. Larry A. Coldren, Scott W. Corzine, Milan L. Mashanovitch, “Diode Lasers and Photonic Integrated Circuits”, John Wiley & Sons, 2 Mar 2012
2. Shun Lien Chuang, “Physics of Photonic Devices”, John Wiley & Sons, 20 Jan 2009.

Location: Tyndall

Type: Fully in-person

Key words: Lasers, photonic integrated circuits (PICs), characterisation, lab

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