# School of Physics Senior Sophister Projects 2026-27
# Physics, Physics and Astrophysics, Nanoscience

June 24, 2026

We look forward to welcoming you to your SS year! As you know you will, during the first 9 weeks of Semester 1 of SS, complete a 20 credit capstone project.

This booklet provides details of the available projects organised by the School of Physics, which we have divided up into pools covering different areas. You can find below lists of the projects in all the areas, along with descriptions for each one. Nanoscience students may also choose from supervisors in the School of Chemistry, which form an additional chemistry pool. The codes you'll need for these supervisors are listed below, and sample projects from them have been provided separately.

You will need to submit 9 choices by entering the corresponding project codes into an online form. You will also be asked to rank the pools. If none of your chosen projects are available you'll be offered the next available project from the pools in the order you rank them.

You may choose no more than 6 projects from any one pool, and 3 from any one supervisor. In addition:

- Physics students may not choose from the astrophysics or chemistry pools.
- Astrophysics students may not choose from the chemistry pool.
- Nanoscience students may not choose from the astrophysics pool.

Projects are all based in Ireland, with most in TCD. There are also astrophysics projects also in the Dublin Institute of Advanced Studies (DIAS) or Armagh Observatory (Armagh).

I hope you enjoy the summer and look forward to meeting you all in September.

Best wishes,

Paul Eastham
Physics SS year head.

# Astrophysics

| Code | | | |
|---|---|---|---|
| AP01 | Samuel Beiler and Johanna Vos | This Old Telescope is Wrong, and We Can Prove It | TCD |
| AP02 | Johanna Vos and Allison McCarthy | Wacky Weather on a World Beyond Our Own | TCD |
| AP03 | Christine Collins and Kate Maguire | Analysing kilonova spectra to identify signatures of heavy elements | TCD |
| AP04 | Johanna Vos and Evert Nasedkin | Model development for exoplanet atmospheres | TCD |
| AP05 | Umut Burgaz and Kate Maguire | FWHM properties of Type Ia supernova spectra in ZTF DR3 sample | TCD |
| AP06 | Tomás Müller Bravo and Kate Maguire | Type Ia supernova twins as a gateway to understanding diversity | TCD |
| AP07 | Kate Maguire | Determining the origin of exotic white dwarf explosions | TCD |
| AP08 | Kate Maguire and Jacco Terwel | Signal smearing due to time-delay effects in supernova interactions | TCD |
| AP09 | Evan Keane | The Crab Pulsar | TCD |
| AP10 | Evan Keane | Setting up an automated all-sky imager for I-LOFAR | TCD |
| AP11 | Evan Keane | Pulsar Surveys with SKA-Low | TCD |

| | | | |
|---|---|---|---|
| AP12 | Neale Gibson | Atmospheres of alien worlds: exploring new tools for high-resolution spectroscopy of exoplanet atmospheres | TCD |
| AP13 | Neale Gibson | Atmospheres of alien worlds: transmission spectroscopy with the James Webb Space Telescope | TCD |
| AP14 | Neale Gibson | Atmospheres of alien worlds: developing new models for exoplanet atmospheres | TCD |
| AP15 | Rossella Anania (Luca Matra) | Characterizing the evolution of planet-forming discs in the sigma-Orionis star-forming region | TCD |
| AP16 | Luca Matra | Exploring the detectability of atomic sulfur emission released by young exocomets with the James Webb Space Telescope | TCD |
| AP17 | Luca Matra | Disk Hunting within the Scorpius-Centaurus Young Stellar Association | TCD |
| AP18 | Mika Holmberg and Maryam Zeroual | Supporting the Jupiter Icy Moons Explorer: Analysis of different spacecraft observations of Earth's space environment | DIAS |
| AP19 | Tim Pearce | Planets carving gaps in cometary belts | TCD |
| AP20 | Tim Pearce | Constraining an unseen planet from a clump in a cometary belt | TCD |
| AP21 | Ryan Begley | Lyman-alpha as a Probe of Ionizing Escape and the Intergalactic Medium | Armagh |
| AP22 | Ryan Begley | Machine Learning Representations of High-Redshift Galaxies | Armagh |
| AP23 | Ryan Begley | Preparing for the Roman Space Telescope Photometric redshifts and galaxy populations | Armagh |
| AP24 | Ryan Begley | Spatially resolved star-formation in the high-redshift Universe with JWST | Armagh |
| AP25 | Laura A. Hayes | Resolving solar flares at the smallest scales with ESA's Solar Orbiter | DIAS |

## Chemistry (for Nanoscience students only)

For School of Chemistry projects you give your choices in terms of the supervisors, using the codes given below. Illustrative projects from these supervisors have been provided separately.

| Code | | |
|---|---|---|
| CRB | Robert Baker | |
| CCD | Colm Delaney | |
| CSD | Sylvia Draper | |
| CPD | Peter Dunne | |
| CLF | Larisa Florea | |
| CYG | Yuri Gunko | |
| CAM | Aidan McDonald | |
| CWS | Wolfgang Schmitt | |
| CCB | Chris Batchelor-McAuley | |
| CPC | Paula Colavita | |

| | |
|---|---|
| CRH | Richard Hobbs |
| CTK | Tobias Kraemer |
| CVN | Valeria Nicolosi |
| CCP | Casey Platnich |
| CGW | Graeme Watson |

## Energy Science

| Code | | | |
|---|---|---|---|
| ES01 | Lewys Jones | Real-time Denoising of Scanning Transmission Electron Microscopy Images | TCD |
| ES02 | David McCloskey | Characterisation of solid state electrochromic thin films for flexible smart window applications | TCD |
| ES03 | David McCloskey | Real-World Coefficient of Performance (COP) of Domestic Heat Pumps in the Irish Climate: Economic and Policy Implications of the SEAI Grant System | TCD |
| ES04 | Stephen Dooley and Bernardo Ballotta | Automated Exploration and Mechanistic Analysis of Xylobiose and Xylotriose Pyrolysis Reaction Networks | TCD |
| ES05 | Stephen Dooley | Molecular Physics Internal Energy Parameters in Multiphysics Models of CO2 Electrolysis Cells: Machine Learned Physics Evaluations | TCD |

## Magnetism and Superconductivity

| Code | | | |
|---|---|---|---|
| MS1 | Plamen Stamenov | Zero-Moment Half-Metallic Ferrimagnets for use in Spintronic Frequency Multipliers | TCD |
| MS2 | Plamen Stamenov | Magnetically-Reconfigurable Diffraction Gratings Constructed of Amorphous Rare-Earth/Transition Metal alloys, for use in Beam-Steering and Magnetic Probabilistic Bit Arrays | TCD |
| MS3 | Plamen Stamenov | Geometrically-Optimized and Shared Memory (GPU)-Parallelized Elliptic Integrals Calculation for Magnetic Field Simulations and Metrological Coil Design | TCD |
| MS4 | Plamen Stamenov and Karsten Rode | Bulk Acoustic Wave (phonon) Coupling of Spintronic Mn2RuxGa Layers Through Thin Non-magnetic Membranes | TCD |

# Materials

| Code | | | |
|---|---|---|---|
| M01 | Kuanysh Zhussupbekov | Atomic-Scale Investigation of Moiré Superlattices in Liquid-Exfoliated 2D Materials | TCD |
| M02 | Jonathan Coleman | Boosting electrical and optical performance of printed 2D materials by doping | TCD |
| M03 | Jonathan Coleman | Electrical and mechanical properties of pressure-treated free-standing thin films of 2D nanosheets | TCD |
| M04 | Jonathan Coleman | Solution-processed photodetectors based on chemically treated 2D semiconducting nanosheet networks | TCD |
| M05 | Jonathan Coleman | Characterising the Electrical Properties of Ultrathin Nanosheet Networks Using Impedance Spectroscopy | TCD |
| M06 | Hongzhou Zhang | AFM Thickness Measurement of Two-Dimensional Materials | TCD |
| M07 | Hongzhou Zhang | Reliable Extraction of Contact Resistance in 2D MoS2 Devices | TCD |
| M08 | Hongzhou Zhang | Machine Learning for Optical Identification of MoS2 Thickness | TCD |
| M09 | Graham Cross, Aaron Sinnott | Does friction depend on how fast you slide? — Prandtl–Tomlinson thermal stick-slip | TCD |
| M10 | Graham Cross, Aaron Sinnott | How much material is removed per unit sliding? — Archard wear law with AFM | TCD |
| M11 | Graham Cross, Aaron Sinnott | Does friction scale linearly with load? — Amontons' Laws in a 2D coating | TCD |
| M12 | Charles Patterson | Excitons in Molecular Crystals | TCD |
| M13 | Cormac McGuinness | "MAD" deposition of large molecular precursors for on-surface synthesis | TCD |
| M14 | Cormac McGuinness | Reduction/oxidation study of metal oxide thin films on ruthenium surfaces – investigation into lowered metal oxide reduction due to bimetallic catalysis | TCD |
| M15 | Cormac McGuinness | The measurement of the reflectance anisotropy spectrum (RAS) arising from penta-silicene nanoribbons formed on Ag(110) | TCD |
| M16 | Cormac McGuinness and Richard Gubo | Development of an Angle-Resolved X-ray Photoelectron Spectroscopy (AR-XPS) Depth Profiling Application | TCD |
| M17 | Igor Shvets | Optical Characterisation of Transparent Conducting Oxides using Spectroscopic Ellipsometry | TCD |
| M18 | Igor Shvets and Varun Ranade | Characterising copper(II) oxide based memristors for neuromorphic computing applications | TCD |
| M19 | Igor Shvets and Amy McGlinchey | Metal-Insulator Transition in Vanadium Oxide | TCD |

| | | | |
|---|---|---|---|
| M20 | Igor Shvets and Igor Chunin | Development of SiO2 Thin-Film Deposition by Electron-Beam PVD for Memristor Applications | TCD |
| M21 | Igor Shvets and Brian Walls | Multilayer p-type transparent conducting oxides: Pristine and nitrogen doped Cu2O | TCD |
| M22 | Jonathan Coleman | Quantifying the relationship between the morphology and mobility of printed nanosheet networks: Towards high performance printed devices | TCD |

## Microscopy and Instrumentation

| Code | | | |
|---|---|---|---|
| MI1 | Kuanysh Zhussupbekov | Surface-Dependent Superconductivity in UTe2: An Atomic-Scale Study | TCD |
| MI2 | Lewys Jones | Vacuum Chamber Molecular Water Contaminant Control | TCD |
| MI3 | Martin Hegner | Biomolecular interaction analysis graphical user interface | TCD |
| MI4 | Martin Hegner | Sensor mechanics investigation during biomolecular recognition | TCD |
| MI5 | Martin Hegner | Quantitatvie recognition of biomolecular interactions | TCD |
| MI6 | Lewys Jones | Design and Simulation of Cryogenic Sample Shield Performance | TCD |

## Photonics

| Code | | | |
|---|---|---|---|
| PH1 | Louise Bradley | Dielectric metasurfaces for emission enhancement | TCD |
| PH2 | Louise Bradley | Coupling a single quantum dot with a single plasmonic nanocavity as a route to single photon emission for quantum applications | TCD |
| PH3 | Louise Bradley | Strong light-matter coupling using plasmonic Au bowtie nanoantennas | TCD |

## Soft and Disordered Matter

| Code | | |
|---|---|---|

| | | | |
|---|---|---|---|
| SM1 | Stefan Hutzler | Experiments with dripping high viscosity liquids | TCD |
| SM2 | Stefan Hutzler | The dynamics of structural transitions in ordered foams | TCD |
| SM3 | Stefan Hutzler | Using statistical methods from econophysics to analyze bubble motion in a two-dimensional foam | TCD |
| SM4 | Matthias Mobius | The shape of sessile droplets | TCD |
| SM5 | Matthias Mobius | Ostwald ripening of evaporating breath figures | TCD |
| SM6 | Ortwin Hess and Illya Tarasenko | Modelling of Electroencephalography (EEG) Signal Propagation Using Quantum Materials | TCD |
| SM7 | Matthias Mobius | Torricelli's law in the viscous limit | TCD |

## Theory and Computation

| Code | | | |
|---|---|---|---|
| T03 | David O'Regan | Accurate modelling of diamond structure semiconductor band gaps | TCD |
| T05 | Pieter Claeys | Belief Propagation for Quantum Dynamics | TCD |
| T07 | Mauro Ferreira | Localisation suppression in low-dimensional quantum systems with correlated disorder | TCD |
| T08 | Mauro Ferreira | Crystalline and amorphous structures in 2D systems: a theory perspective | TCD |
| T12 | John Goold and Mattia Moroder | Numerical optimization of dissipative preparation protocols for topological states | TCD |
| T14 | Charles Patterson | Learning to Solve Physical Problems using High Performance Computing Methods | TCD |
| T15 | Charles Patterson | Parameter Optimisation using Linear Least Squares, LASSO and Ridge Regression Methods | TCD |
| T16 | Phillip Christie | Analysis of brain connectome | TCD |
| T17 | Phillip Christie | Analysis of critical phase transitions in very large digital integrated circuits | TCD |
| T18 | Phillip Christie | Theoretical analysis of critical phase transitions in digital integrated circuits | TCD |
| T19 | John Goold and Artur M. Lacerda | Gibbs Sampling for phase-modulated Neural Quantum States | TCD |
| T20 | John Goold and Artur M. Lacerda | Shortcuts to adiabaticity in open quantum systems: purity leakage in dark spaces | TCD |
| T23 | Cormac McGuinness | Simulating interactions and electronic structure of metal-porphyrin nanostructures | TCD |
| T24 | Paul Eastham | Efficient qubit reset beyond the Born-Markov approximation | TCD |
| T29 | Stefano Sanvito | ML models for materials designed by AutoResearch | TCD |
| T30 | Stefano Sanvito | Creating an atomic DFT code with AI | TCD |

| | | | |
|---|---|---|---|
| T31 | Stefano Sanvito | Phase stability predictions with foundational force fields | TCD |
| T32 | Plamen Stamenov | Real-Time Scientific Visualization – Volume Rendering of Scalar and Vector Fields – Towards an Ultra-Light and User- and Hardware-Friendly Display Engine | TCD |

# This Old Telescope is Wrong, and We Can Prove It

Dr. Samuel Beiler and Prof. Johanna Vos

Before the James Webb Space Telescope, the premier infrared telescope was the Spitzer Space Telescope. It was used to detect exoplanet weather, saw the birth of new stars, and characterized hundreds of the coldest products of star formation called brown dwarfs. Working in space and actively cooled, it was the one of the only instruments capable of observing from 3-5 microns with high sensitivity, and it collected an untold amount of images over its nearly two decades of service. Spitzer transformed astronomy, yet unbeknownst to everyone, something was wrong.

With the launch of the James Webb Space Telescope (which can observe similar wavelength ranges) we found that its results did not line up with Spitzer. One of Spitzer's instruments was consistently brighter than JWST. Unfortunately, there are not enough overlapping targets to full characterize the discrepancy and determine what is wrong and how far reaching the consequences are. **This project will aim to use a suite of data from the newly launched SPHEREx mission to characterize the Spitzer issue and discover its root cause.** Doing so may have far reaching effects on all corners of infrared astronomy.

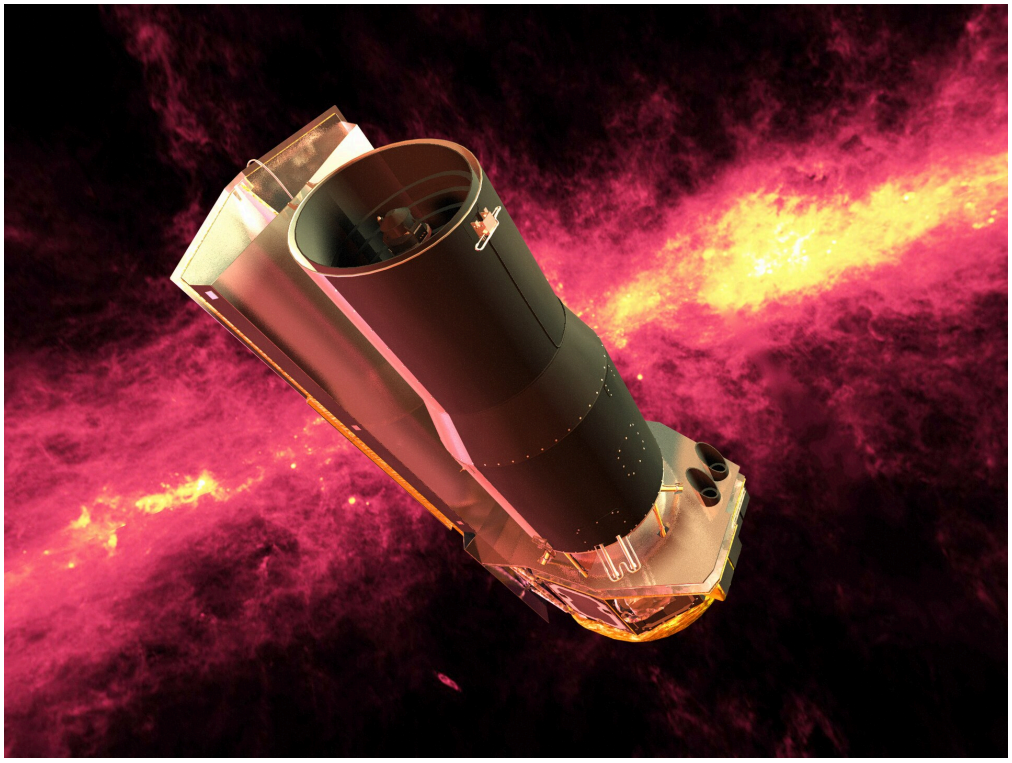


Figure 1: Artists Depiction The Spitzer Space Telescope

# Wacky Weather on a World Beyond Our Own

Dr. Allison McCarthy and Prof. Johanna Vos
mccara45@tcd.ie

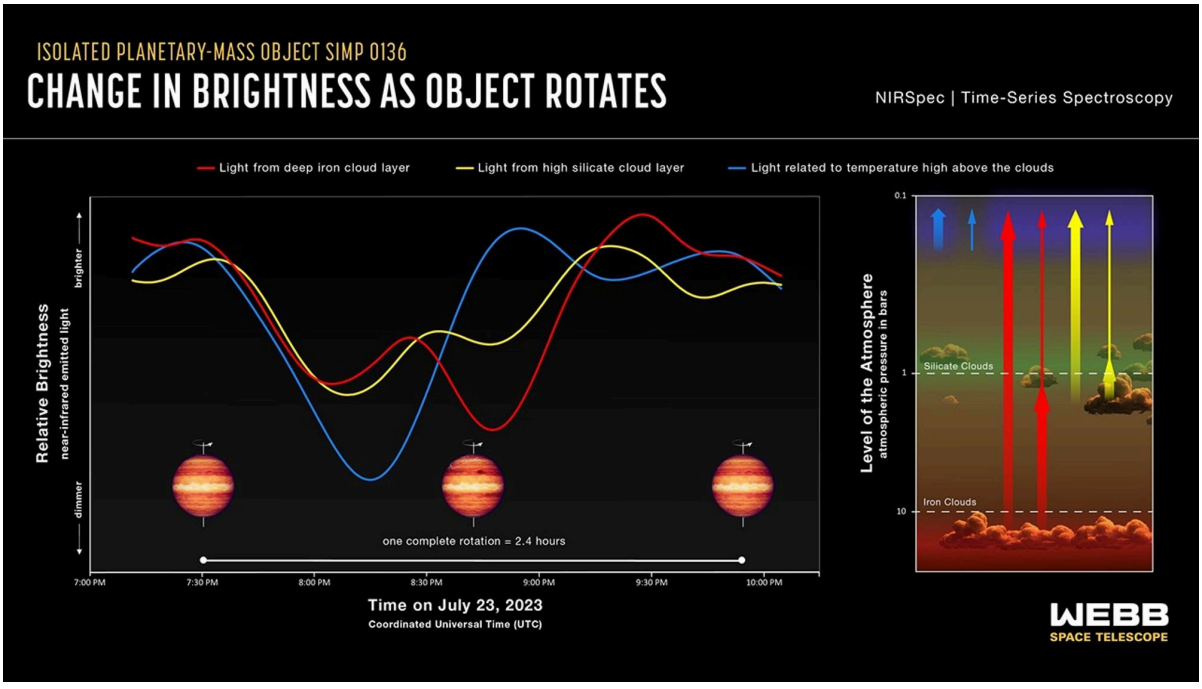
Exometeorology – the study of atmospheric processes and phenomena on worlds beyond our solar system – has rapidly evolved from a non-existent field, 25 years ago, to one of the most exciting and groundbreaking fields in astronomy. Now, with the expansive wavelength coverage and high precision of JWST, we are better equipped than ever to investigate the physics and chemistry which drive the evolution of the atmospheric structure of extrasolar worlds.

Brown dwarfs and planetary-mass objects, which bridge the gap between the smallest of stars and the largest of planets, are the ideal laboratories for exometeorological studies. These objects offer valuable insight into the atmospheric structure of exoplanets. But, without the blinding light of a bright host star, brown dwarfs and planetary-mass objects are easier to observe.

Our current understanding of the evolution of the atmospheric structure of giant exoplanets and their analogs is based on four main mechanisms: clouds, chemical abundances, hot spots, and aurorae. Until we can accurately disentangle the signatures of all variability mechanisms on isolated objects, we cannot properly characterize and model extrasolar atmospheres. Now, in the era of JWST, spectroscopic monitoring programs provide immense amounts of data across a broad range of wavelengths. This project will use data from JWST to investigate the temporal variations in the atmosphere of a brown dwarf and use state-of-the-art models to determine which of the four main mechanisms are shaping the weather on this extrasolar world.

**Further Reading:**

McCarthy et al. (2025): https://ui.adsabs.harvard.edu/abs/2025ApJ...981L..22M/abstract
Biller (2017): https://ui.adsabs.harvard.edu/abs/2017AstRv..13....1B/abstract



# Analysing kilonova spectra to identify signatures of heavy elements

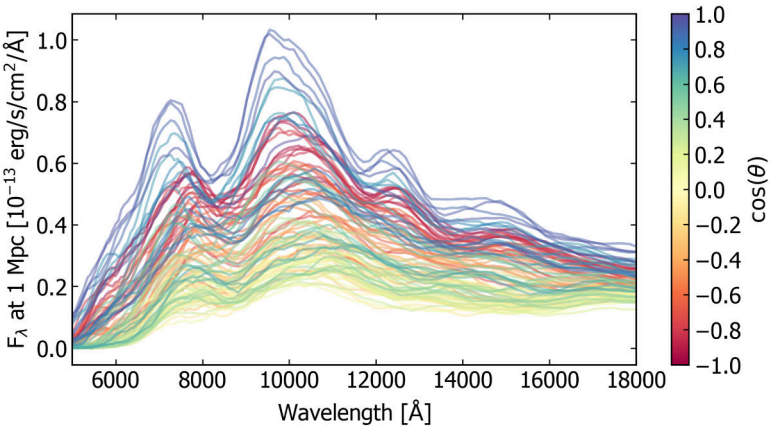
Christine Collins, Kate Maguire

Background

When neutron stars collide the heaviest elements in the Universe are formed. These explosive events release enormous amounts of energy, causing a burst of light known as a kilonova. By studying these objects we can understand where our heavy elements such as gold and platinum are produced. The first ever confirmed kilonova, AT2017gfo, was observed in 2017, however, understanding the observed spectra is still ongoing. Only a handful of elements have been identified in the spectra and the amounts of these elements produced is highly uncertain.

We can interpret the observations and identify the elements produced by carrying out kilonova radiative transfer simulations to predict what the spectra of a known composition would look like to an observer.

Project aims




The figure shows simulated spectra from a 3D kilonova model viewed from 100 different directions. The aim of this project is to analyse kilonova simulations like these using Python. A key question in kilonova research is how much lanthanide material is produced in the explosion. Lanthanides are a group of heavy elements with atomic numbers 57 to 71, and they strongly influence the appearance of kilonova spectra.

In these simulations, the lanthanide fraction of the ejecta is known. The goal of the project is therefore to identify features in the simulated spectra that correlate with lanthanide fraction, and to investigate whether these spectral signatures could be used to estimate lanthanide abundances in observed kilonovae.

# Model Development for Exoplanet Atmospheres

Dr. Evert Nasedkin & Prof. Johanna Vos

April 17, 2026

This project provides a student with an open-ended opportunity to contribute to `petitRADTRANS`[1], a widely used python package for modelling exoplanet atmospheres. These models use one-dimensional radiative transfer to calculate the emission or transmission spectrum of the atmosphere. A typical use for this models is to fit observational data, which can require the computation of $10^6 - 10^7$ forward models.

During this project, the student will identify a topic of interest from one of:

1. Numerical methods for radiative transfer
2. Parameterising time-dependent atmospheric phenomena
3. Machine learning to predict atmospheric properties

Each of these sub-topics represents an active area of research, and will be key developments for the next generation of atmospheric characterisation. The first topic would be best suited for a student interested in lower-level programming and numerical methods, and would involve the adaptation of novel schemes for solving the equations of radiative transfer for the specific case of exoplanet atmospheres. The second topic would design new parameterisations of the atmospheric state, with the goal of inferring dynamical properties such as the physical scale of weather features or the wind speed in the atmosphere. The third project would optimise the neural network architecture for simulation based inference, training models and deploying them to characterise a range of exoplanet or brown dwarf atmospheres.

[1] `https://petitradtrans.readthedocs.io/en/latest/`

**Spectral properties of Type Ia supernova spectra in ZTF DR3 sample**

**Dr. Umut Burgaz and Prof. Kate Maguire (School of Physics)**
burgazu@tcd.ie, kate.maguire@tcd.ie

Supernovae are stellar explosions that experience a rapid and immense increase in brightness within days, followed by a gradual fading over months. Type Ia supernovae (SNe Ia) are widely believed to result from the high-energy thermonuclear detonation of a carbon-oxygen white dwarf in a binary system.

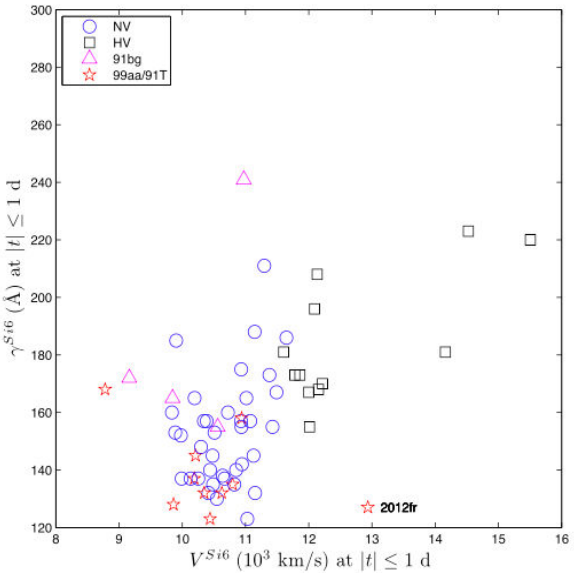



*Fig 1:* Si II λ6355 velocity versus FWHM for SNe Ia.

SNe Ia can be classified into two spectral subtypes based on the Si II λ6355 expansion velocity near peak brightness as high velocity (HV) SNe Ia and normal velocity (NV) SNe Ia [1]. However, the velocity alone may not capture the full diversity of SN Ia spectra. Recent work has shown that the width of absorption features may also contain important physical information (Fig. 1), reflecting the velocity spread and temperature structure of the ejecta [2]. As interest in transient astronomy grows, large-scale surveys like the Zwicky Transient Factory (ZTF) are providing unprecedented data for studying these events.

In this project, we will use the Zwicky Transient Facility (ZTF) DR3 Type Ia supernova sample [3] to investigate the spectral properties of SNe Ia, focusing on the Si II λ6355 absorption feature. Using an existing catalogue of measurements, we will examine how the width (FWHM) of this feature correlates with expansion velocity and spectroscopic subtype, and whether it provides additional information beyond the standard HV/NV classification. The next step will be to explore the diversity of SNe Ia by comparing subsets with different properties and identifying similarities and differences between them. As an extension, Principal Component Analysis (PCA) will be used to explore whether combinations parameters can improve the classification of SNe Ia.

Understanding the diversity of SNe Ia is important for both astrophysics and cosmology. Variations in spectral properties may reflect differences in explosion physics or progenitor systems, and can introduce systematic uncertainties in cosmological studies. Therefore, identifying additional spectroscopic indicators beyond velocity can improve the selection and calibration of SN Ia samples.

Python will be used throughout the project, so good programming skills, preferably in Python, are highly recommended.

**References:** [1] Wang, X., et al., 2009, ApJ, 699, 139; [2] Zhao, X., et al., 2026, RAA, 26, 065002; [3] Burgaz U., et al., 2026, in prep.

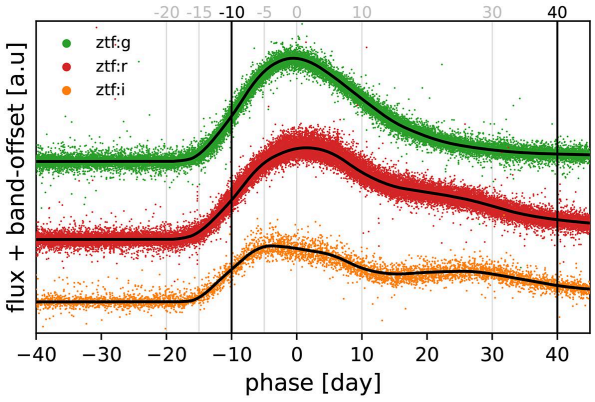
# Type Ia supernova twins as a gateway to understanding diversity

**Dr. Tomás Müller Bravo, t.e.muller-bravo@tcd.ie**
**Prof. Kate Maguire, kate.maguire@tcd.ie**

**Background**: Type Ia supernovae (SNe Ia) are thermonuclear explosions of white dwarfs in binary systems and key tools for measuring cosmological distances and the expansion history of the Universe. Their use as “standardisable candles” relies on empirical relations between light curve shape, colour, and luminosity, as implemented in models such as SALT2. However, SNe Ia show significant diversity in both photometric and spectroscopic properties, introducing systematic uncertainties in cosmological measurements.

An alternative approach is the concept of “supernova twins,” where pairs (or groups) of SNe Ia with nearly identical observational properties are identified. Such twins have been shown to reduce scatter in intrinsic luminosity compared to standard methods [1]. While traditional twin studies rely on spectroscopic time series, modern wide-field surveys now provide large photometric datasets that enable the development of **photometric twinning** techniques, offering a scalable way to probe SN Ia diversity and improve distance measurements.

**Project aim**: This project will identify and analyse photometric twins of Type Ia supernovae using optical light curves from the Zwicky Transient Facility (ZTF [2]). A homogeneous sample of spectroscopically confirmed SNe Ia with well-sampled g- and r-band light curves will be used (Fig 1.). The student will develop a quantitative similarity metric to compare multi-band light curves and identify “twin” objects with highly similar photometric evolution. These twins will be analysed to determine whether they form a physically meaningful structure within the SN Ia population.




The project will test whether photometric twins show reduced scatter in peak luminosity compared to standardisation methods based on SALT2. Relationships between twin similarity and other properties will also be explored, assessing whether twinning captures information beyond standard light-curve parameters.The analysis will be performed in Python using standard scientific libraries. Statistical techniques will be used to assess the robustness of the twin identification, and optional extensions may include clustering methods to visualise SN Ia diversity. The results are relevant for future large-scale surveys such as the Legacy Survey of Space and Time (LSST [3]), where scalable methods for supernova characterisation will be essential.

**Fig 1.**: SN Ia light curves from the ZTF sample compared to a mean SALT2 model [2].

**References:**

[1] Boone, Aldering, Antilogus et al. ApJ, 912, 70 (2021)
[2] Rigault, Smith, Goobar et al. A&A, 694, A1 (2025)
[3] Ivezić, Kahn, Tyson et al. ApJ, 873, 111 (2019)

# Determining the origin of exotic white dwarf explosions

**(Prof. Kate Maguire, kate.maguire@tcd.ie)**

**Background:** Type Ia supernovae are some of the most energetic explosions in the Universe and are essential as probes of the mysterious quantity dark energy that makes up 70% of the mass energy of the Universe. Despite their importance, the physical mechanisms that trigger these explosions remain uncertain, with multiple explosion scenarios likely contributing to the observed population. A key challenge is to connect theoretical explosion models with observed supernova samples to assess their validity.

**Recent breakthroughs:** Recent work has highlighted *violent white dwarf mergers* as a promising pathway for producing certain peculiar Type Ia supernovae (e.g. Dimitriadis et al. 2025; Pakmor et al. 2026). These models predict highly asymmetric explosions, meaning that observed properties depend strongly on viewing angle. Notably, for some orientations, the models produce spectra with unusually weak silicon features, that are distinct from the strong silicon lines seen in Type Ia supernovae (Fig. 1). This raises a critical question: if such explosions occur in nature, where are they in observed samples? Their absence may indicate either that the models are incomplete or that such events have been misclassified due to their atypical spectral signatures. Resolving this is essential for evaluating the viability of the violent merger scenario.

**Project aim:** This project will test the hypothesis that supernovae arising from violent mergers already exist within current datasets but have been misidentified. Using data from the Zwicky Transient Facility (ZTF https://www.ztf.caltech.edu/), one of the largest and most comprehensive transient surveys to date, the student will develop novel analysis techniques to identify candidate events. The approach will involve comparing theoretical predictions from violent merger simulations with observed light curves and spectra, with a focus on identifying objects that lack strong silicon features. By systematically searching the ZTF sample, the project aims to determine whether these elusive events are present and, if so, quantify their occurrence rate. Detecting such events would provide strong support for violent merger models. Conversely, a robust non-detection would place stringent constraints on these models, potentially ruling them out as a significant contributor to the observed population.

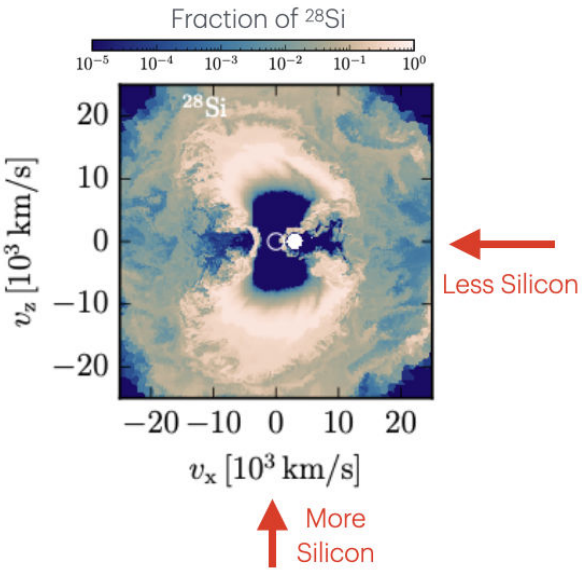



*Figure 1: Adapted from Pakmor et al. (2026). Slice through in the xz plane of a 3D 'violent merger' explosion simulation, showing the fractional abundance of $^{28}$Silicon. Viewing the explosion from the right-hand side results in observations with low amounts of visible Silicon. Do supernovae like this exist but have been missed?*

**References:** Dimitriadis et al., 2023, MNRAS, 521, 1162, Hoogendam et al., 2024, 966, 139, Pakmor et al., 2026, A&A, 706, 239

# Signal smearing due to time-delay effects in supernova interactions

## Background:

Current large-scale surveys such as the Zwicky Transient Facility (ZTF) and the Asteroid Terrestrial-impact Last Alert System (ATLAS), as well as the upcoming Legacy Survey of Space and Time (LSST) it has become possible to accurately and periodically observe the same part of the sky over timeframes of years. Repeating observations every few days (2 - 3 day cadence) has proven extremely successful in discovering large amounts of supernovae (SNe) and other transient events in the universe, with hundreds of new events being discovered each year. Each of these has been observed for years before and/or after the transient was first detected, providing rich datasets that could contain faint signals hiding in the noise. Recently, this has been used to find signs of interaction between SN ejecta and circumstellar material (CSM) months to years after the explosion (Terwel et al. 2025a,b,c). This CSM is thought to come from the SN progenitor system, which could have lost the material through a variety of processes such as a stellar wind, episodic mass loss, or binary interaction. CSM therefore holds vital clues about the star(s) in the progenitor system before the SN. The delay between the SN and the onset of CSM interaction suggests that the CSM resides at a large distance ($> 10^{16}$ cm) from the explosion site, and that it has been ejected a long time ago. The time evolution of the observed CSM signal therefore not only depends on CSM properties such as its shape and density, but the time-delay between light coming from the near and far sides of the CSM should also be taken into account as it will smear features in the observed signal.

## Project aim:

The aim of this project is to study the smearing effects of time-delay on CSM signals. To do this a description is needed that transforms an assumed CSM interaction model in the SN frame to the observed signal evolution in the observer frame. Starting with a simple shell model in 2D and 3D, this description can then be refined to describe more complex CSM configurations such as a thin disk, a thick torus, or a non-constant density profile. These can then be used to answer questions such as: 1) Is it possible to use the observations to distinguish between CSM configurations or does the time-delay smear everything out to look the same? 2) For an observed Ia-CSM, can we find one or more CSM configurations that can reproduce the observed light curve? 3) Assuming that there are observable differences between two CSM models, will the observing strategy of ZTF or LSST be adequate to differentiate between these models? These results are useful to optimise detection and follow-up strategies of these rare events, and can be used to infer information about the CSM configuration from their light curve shape.

## References:

Terwel et al., 2025a, A&A, 694, A11, Terwel et al., 2025b, A&A, 697, A143, Terwel et al., 2025c, A&A, 702, A21
https://ui.adsabs.harvard.edu/abs/2025A%26A...694A..11T/abstract
https://ui.adsabs.harvard.edu/abs/2025A%26A...697A.143T/abstract
https://ui.adsabs.harvard.edu/abs/2025A%26A...702A..21T/abstract

## The Crab Pulsar

Prof Evan Keane
evan.keane@tcd.ie

Pulsars are rapidly rotating neutron stars, dotted around the Galaxy, which emit lighthouse-like beacons from their polar regions as they spin. This sweeping clock-like signal enables astronomers to study a plethora of fundamental physics, impossible to test in an Earth-bound laboratory. The Crab pulsar is the exemplar object for studying the extreme physics of neutron stars; also for using pulsar signals to study the environment in the Crab nebula, the remnant of the supernova wherein this star formed in 1054 CE.

Data collected over the past few years observing the Crab with the Irish LOFAR station [1], at TCD's Rosse Observatory, constitutes the best collection of data on the source [2]. As of April 2026, over one million giant pulses of emission have been detected. These data give us an insight to the extreme electromagnetic processes occurring near the star [3]. The light from the star traverses the Crab nebula which imparts its characteristics on the light; this can be disentangled to understand the structure of the nebula [4]. This project involves data analysis (in a unix environment) and theoretical interpretation of this large data collection with a view to understanding the emission processes in the Crab, and the interstellar 'weather' in the nebula. This project will likely involve one or two trips to the Observatory.

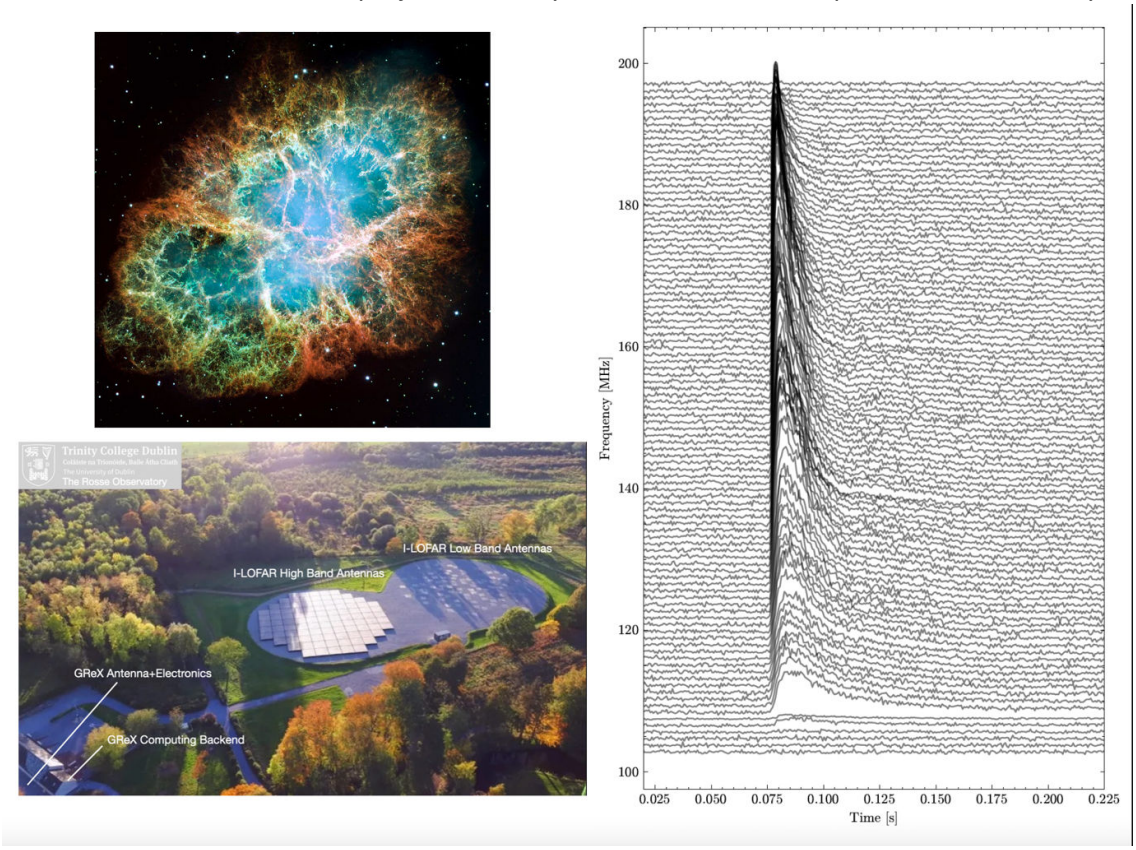



Fig. 1 : Top Left: Hubble Space Telescope image of the Crab Nebula. Bottom Left: Aerial view of the Rosse Observatory showing the I-LOFAR telescopes where the data for this project has been collected. Right: Example pulse In a 0.2-second snippet from the I-LOFAR data.

### References

[1] "First results from the REAL-time Transient Acquisition backend (REALTA) at the Irish LOFAR station", Murphy et al., *A&A*, **655**, 16 (2021).
[2] "100 000 Crab giant pulses at 215 MHz detected with an SKA-Low prototype station"", Sokolowski et al., *PASA*, **42**, 145 (2025).
[3] "Nanosecond radio bursts from strong plasma turbulence in the Crab pulsar", Hankins et al., *Nature,* **422**, 141 (2003).
[4] "Frequency-dependent Dispersion Measures and Implications for Pulsar Timing", Cordes et al., *ApJ*, **817**, 16 (2016).

**Setting up an automated all-sky imager for I-LOFAR**

Prof Evan Keane
evan.keane@tcd.ie

TCD's Rosse Observatory hosts the Irish LOFAR station [1], which consists of 2 telescopes – a low-band array operating in the ~10-90 MHz range, and a high-band array operating in the ~110-240 MHz range. It routinely observes the sun (during daytime) and pulsars [2] with occasional studies of flare stars, auroral emission from solar system planets and searches for technosignatures from exoplanetary systems [3].

It is capable of, but rarely does, so-called 'all-sky' imaging whereby the signals from each of the 92x2 antennas of a given array are correlated (as opposed to added) to make a low-resolution but wide field-of-view radio image of the sky. Using the low-band the field of view is very large and we can see more or less to the physical horizon. This is employed principally to identify sources of local interference when they arise, but it is not yet used for scientific research despite the vast potential [4]. Adding this feature would open a new window of scientific exploration at the Observatory.

This project involves setting up an automated analysis pipeline to create all-sky images automatically each night, configurable to be sensitive to transient events from the terrestrial (e.g. meteors) to the solar system (e.g. radio bursts from the Jupiter-Io system) to the Galactic (bursts from flare stars). The project is primarily one of data analysis and will involve shell scripting and python (or other languages as preferred) in a Unix environment. It might involve one or two trips to the Rosse Observatory, in Birr Co. Offaly.

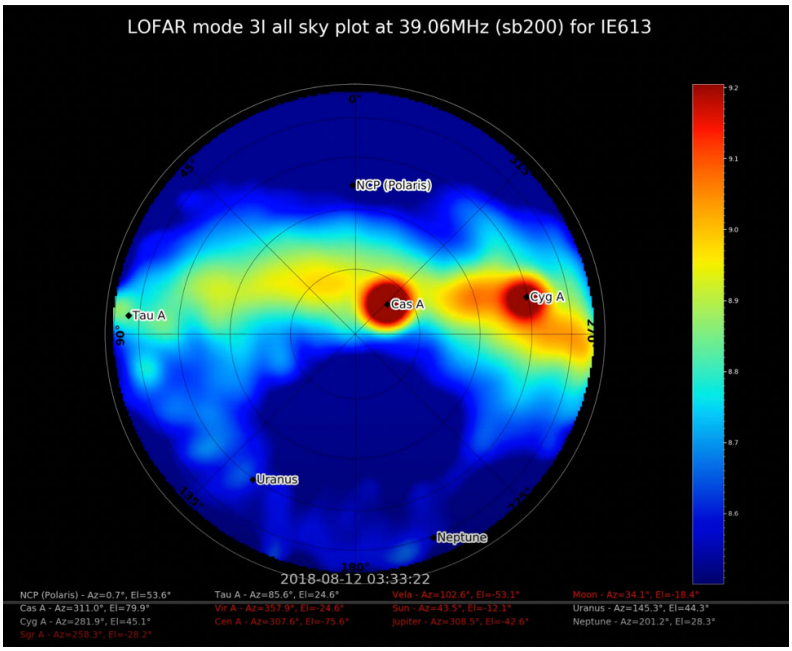



Fig. 1 : An example all-sky Stokes I total intensity image taken at 39.06 MHz using the I-LOFAR low band antennas, a snapshot from a multi-hour observing campaign [4]. Visible are the Galactic plane and several very bright 'A Team' sources, Taurus A, Cygnus A and Cassiopeia A.

**References**

[1] "LOFAR: The LOw-Frequency ARray", van Haarlem et al., *A&A*, **556**, 53 (2013).
[2] "Long-term timing results of ecliptic pulsars observed with I-LOFAR", Susarla et al., *A&A*, **698**, 248 (2025)
[3] "A Simultaneous Dual-site Technosignature Search Using International LOFAR Stations" Johnson et al., *AJ*, **166**, 15 (2023).
[4] Somewhat similar system to that envisioned, deployed at the LWA in New Mexico: https://leo.phys.unm.edu/~lwa/lwatv.html
[5] A (sped-up) 10-hour track of the sky with I-LOFAR at 39.06 MHz: https://www.youtube.com/watch?v=E0_ugUHa0vc

**Pulsar Surveys with SKA-Low**

Prof Evan Keane
evan.keane@tcd.ie

Pulsars are rapidly rotating neutron stars, dotted around the Galaxy, which emit lighthouse-like beacons from their polar regions as they spin. This sweeping clock-like signal enables astronomers to study a plethora of fundamental physics, impossible to test in an Earth-bound laboratory. Principle among these are gravitational studies in the strong-field and radiative regimes. Only ~3800 of the estimated 200,000 pulsars estimated in the Milky Way have so far been detected [1]. Astronomers are keen to find ever more extreme binaries to test General Relativity against alternative theories [2], and to discover ever more millisecond pulsars for more sensitive and precise gravitational wave detections [3]

SKA-Low is currently under construction in Western Australia; it will be the biggest telescope in the world even when partially complete. It constitutes a massive leap over existing instruments operating in the frequency range, such as LOFAR in Europe or the GMRT in India. SKA-Low is particularly suited to pulsar surveys due to its sensitivity and field-of-view [4, 5]. This project involves simulations and theoretical work, modelling different pulsar survey search strategies. It examines the question of **how best to search for pulsars with SKA-Low?** This question will also be considered re: pilot survey strategies using the already partially deployed 'array assembly 2', available for use in 2027.

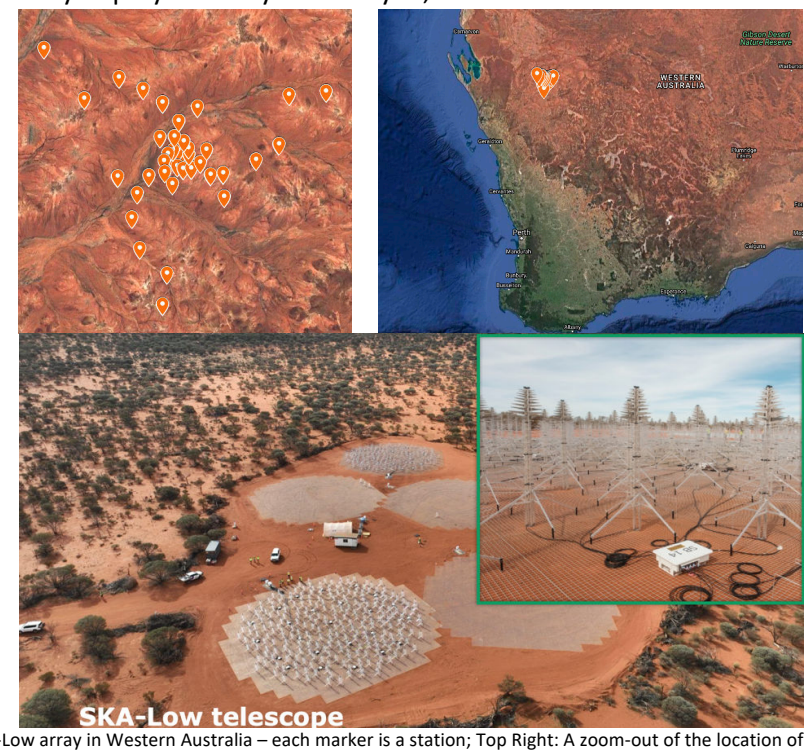



Fig. 1 : Top Left: SKA-Low array in Western Australia – each marker is a station; Top Right: A zoom-out of the location of SKA-Low; Bottom: Two of the first deployed stations; inset showing a close-up of a station of 256 'christmas tree' antennas.

**References**

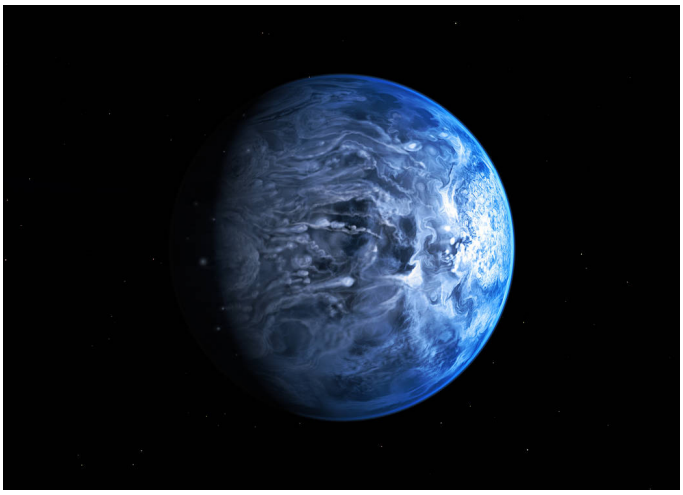
[1] ATNF Pulsar Catalogue: atnf.csiro.au/people/pulsar/psrcat
[2] "Strong-Field Gravity Tests with the Double Pulsar", Kramer et al., *PhysRevX*, **11**, 041050 (2021).
[3] "The second data release from the European Pulsar Timing Array. III. Search for gravitational wave signals", Antoniadis et al., *A&A*, **678**, 50 (2023).
[4] "Pulsar Science with the SKA", Keane, *IAU Symposium Proceedings,* **337**, 158 (2018).
[5] "A Square Kilometre Array Pulsar Census", Keane et al., *OJAp*, **8 Supplement**, 1 (2025).

# Atmospheres of alien worlds: exploring new tools for high-resolution spectroscopy of exoplanet atmospheres

**Prof. Neale Gibson**
n.gibson@tcd.ie

**Research Project Description:**

In the last decades, radial velocity and transit surveys have made enormous progress in detecting the population of exoplanets in our Galaxy, yet we still know very little about the planets themselves. Transiting planets, those that periodically eclipse their host stars, play a special role in our understanding of exoplanets, as they allow us to characterise their atmospheres in detail using techniques such as emission and transmission spectroscopy. For example, transmission spectroscopy is a measurement of the effective planetary radius as a function of wavelength. As starlight filters through the upper atmosphere of a planet during transit, this leaves a spectral imprint that can reveal the chemical composition and physical properties of an exoplanet's atmosphere.



Artists impression of exoplanet HD 189733 b, “Rains of Terror”. Credit: ESO / M. Kornmesser

This project will use a technique called Doppler-resolved transmission spectroscopy. This uses high-resolution time-series spectra during transit to try and disentangle light from the star and planet by exploiting the large Doppler shift of the exoplanet's spectral signature compared to its host star. The project will use optical an/or infrared data from ESO’s Very Large Telescope to search for atomic or molecular species in an exoplanet atmosphere, as well as potentially exploring new machine-learning and/or statistical tools to recover information on the planet's atmosphere. Note that the exact data and methods proposed are subject to change, as the field of exoplanet atmospheres is rapidly evolving.

**References:**

Below are some references to help learn more. The top three references are review articles in the area of exoplanets and exoplanet atmospheres, and are a good place to start. The remainder are articles from our group providing more specific examples in the area. Please feel free to contact me if you have any questions.

Winn (2010), “Transits and Occultations”, https://arxiv.org/abs/1001.2010

Crossfield (2015), “Observations of Exoplanet Atmospheres”, PASP, Volume 127, 956

Birkby (2018), “Exoplanet Atmospheres at High Spectral Resolution”, https://arxiv.org/abs/1806.04617

Gibson et al. (2012), “A Gaussian process framework for modelling instrumental systematics: application to transmission spectroscopy”, Monthly Notices of the Royal Astronomical Society, Volume 419, Issue 3, pp. 2683-2694

Gibson et al. (2020), “Detection of Fe I in the atmosphere of the ultra-hot Jupiter WASP-121b, and a new likelihood-based approach for Doppler-resolved spectroscopy”, Monthly Notices of the Royal Astronomical Society, Volume 493, Issue 2, p.2215-2228

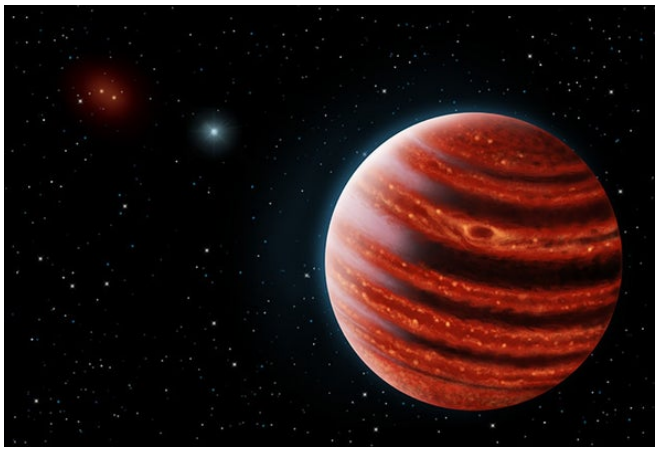
Wilson, Gibson et al. (2021), “Gemini/GMOS Optical Transmission Spectroscopy of WASP-121b: signs of variability in an ultra-hot Jupiter?”, MNRAS, in press

# Atmospheres of alien worlds: transmission spectroscopy with the James Webb Space Telescope

**Prof. Neale Gibson**
n.gibson@tcd.ie

**Research Project Description:**

In the last decades, radial velocity and transit surveys have made enormous progress in detecting the population of exoplanets in our Galaxy, yet we still know very little about the planets themselves. Transiting planets, those that periodically eclipse their host stars, play a special role in our understanding of exoplanets, as they allow us to characterise their atmospheres in detail using techniques such as emission and transmission spectroscopy. For example, transmission spectroscopy is a measurement of the effective planetary radius as a function of wavelength. As starlight filters through the upper atmosphere of a planet during transit, this leaves a spectral imprint that can reveal the chemical composition and physical properties of an exoplanet's atmosphere.



Artists impression of exoplanet 51 Eridani b: Credit: Danielle Futselaar and Franck Marchis/SETI Institute/Gemini Planet Imager

This project will use a technique called transit (transmission) spectroscopy using time-series spectro-photometry. This uses precise measurements of exoplanet transits as a function of wavelength to determine the wavelength-dependent absorption from the planet's atmosphere. The project will use archival data from the James Webb Space Telescope or the Very Large Telescope to search for atomic/molecular features in an exoplanet atmosphere, and/or explore the use of new machine-learning and/or statistical tools to recover information on the planet's atmosphere. Note that the exact data and methods proposed are subject to change, as the field of exoplanet atmospheres is rapidly evolving.

**References:**

Below are some references to help learn more. The top three references are review articles in the area of exoplanets and exoplanet atmospheres, and are a good place to start. The remainder are articles from our group providing more specific examples in the area. Please feel free to contact me if you have any questions.

Winn (2010), "Transits and Occultations", https://arxiv.org/abs/1001.2010

Crossfield (2015), "Observations of Exoplanet Atmospheres", PASP, Volume 127, 956

Birkby (2018), "Exoplanet Atmospheres at High Spectral Resolution", https://arxiv.org/abs/1806.04617

Gibson et al. (2012), "A Gaussian process framework for modelling instrumental systematics: application to transmission spectroscopy", Monthly Notices of the Royal Astronomical Society, Volume 419, Issue 3, pp. 2683-2694

Gibson et al. (2020), "Detection of Fe I in the atmosphere of the ultra-hot Jupiter WASP-121b, and a new likelihood-based approach for Doppler-resolved spectroscopy", Monthly Notices of the Royal Astronomical Society, Volume 493, Issue 2, p.2215-2228

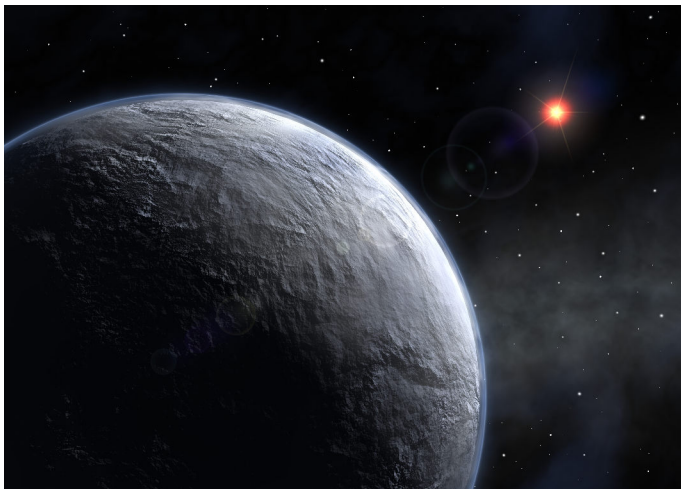
Wilson, Gibson et al. (2021), "Gemini/GMOS Optical Transmission Spectroscopy of WASP-121b: signs of variability in an ultra-hot Jupiter?", MNRAS, in press

# Atmospheres of alien worlds: developing new models for exoplanet atmospheres

**Prof. Neale Gibson**
n.gibson@tcd.ie

**Research Project Description:**

In the last decades, radial velocity and transit surveys have made enormous progress in detecting the population of exoplanets in our Galaxy, yet we still know very little about the planets themselves. Transiting planets, those that periodically eclipse their host stars, play a special role in our understanding of exoplanets, as they allow us to characterise their atmospheres in detail using techniques such as emission and transmission spectroscopy. For example, transmission spectroscopy is a measurement of the effective planetary radius as a function of wavelength. As starlight filters through the upper atmosphere of a planet during transit, this leaves a spectral imprint that can reveal the chemical composition and physical properties of an exoplanet's atmosphere.



Artists impression of an icy exoplanet. Credit: ESO. (Though this project will most likely look at gas giants.)

Our group regularly uses data from ESO's Very Large Telescope and the James Webb Space Telescope to observe and understand the atmospheres of transiting planets. To interpret these data we typically use simple 1D plane parallel model atmospheres (a single column of atmosphere) to simulate an exoplanet spectrum. On the other hand, General Circulation Models (GCMs; effectively the same models that are used to model Earth's weather and climate) model the spatial and temporal variation on the surface of the planet. The latter are too complex to apply to model inference, whereas the data has already exceeded our ability to model them in 1D. This project will aim to bridge the gap between simple 1D models and complex 3D models using one of two approaches; 1) by integrating multiple 1D models into a single model capable of modelling the 3D surface of a planet for inference or 2) by developing a spectral emulator using a machine learning approach over a grid of forward models to dramatically speed up the computation of simple 1D models. The exact approach will depend on the student's interests plus the current data being analysed within the group.

***Note that this project is only suitable for a TP student who has done the JS module PYU33A03 (Stellar and Galactic Structure) or has other suitable experience (contact me if in doubt).***

**References:**

Below are some references to help learn more. The top three references are review articles in the area of exoplanets and exoplanet atmospheres, and are a good place to start. The remainder are articles from our group providing more specific examples in the area. Please feel free to contact me if you have any questions.

Winn (2010), "Transits and Occultations", https://arxiv.org/abs/1001.2010

Crossfield (2015), "Observations of Exoplanet Atmospheres", PASP, Volume 127, 956

Birkby (2018), "Exoplanet Atmospheres at High Spectral Resolution", https://arxiv.org/abs/1806.04617

Gibson et al. (2012), "A Gaussian process framework for modelling instrumental systematics: application to transmission spectroscopy", Monthly Notices of the Royal Astronomical Society, Volume 419, Issue 3, pp. 2683-2694

Gibson et al. (2020), "Detection of Fe I in the atmosphere of the ultra-hot Jupiter WASP-121b, and a new likelihood-based approach for Doppler-resolved spectroscopy", Monthly Notices of the Royal Astronomical Society, Volume 493, Issue 2, p.2215-2228

Wilson, Gibson et al. (2021), "Gemini/GMOS Optical Transmission Spectroscopy of WASP-121b: signs of variability in an ultra-hot Jupiter?", MNRAS, in press

# Characterizing the evolution of planet-forming discs in the sigma-Orionis star-forming region

*Dr. Rossella Anania,* ananiar@tcd.ie

*Prof. Luca Matrà,* lmatra@tcd.ie

Planets originate in disc-like structures of gas and dust around young stars. Understanding the main processes driving the evolution of protoplanetary discs is therefore essential to unveil how planets form. Since most young stars are born in massive clusters, the stellar formation environment plays a fundamental role in shaping disc evolution and, ultimately, planet formation.

Massive stars (i.e., of spectral type O and B) emit intense UV radiation. When this radiation heats the outermost regions of protoplanetary discs, which are weakly gravitationally bound to the central star, produces an outside-in depletion of material. This process, known as external photoevaporation, significantly reduces disc mass, size, and lifetime, affecting the efficiency of planet formation.

Sigma-Orionis is the closest star-forming region exposed to UV radiation fields typical of planet-forming environments in the Galaxy, and similar to those experienced by the early Solar System. This cluster offers a unique opportunity to investigate environmentally driven disc evolution. At its center lies the massive star sigma-Orionis (which gives the name to the cluster), illuminating the surrounding protoplanetary discs. We expect the discs closer to the center to be smaller and less massive compared to those in the outskirts.

This project will simulate the evolution of protoplanetary discs under the effect of external photoevaporation using a 1D numerical disc evolution code. Comparing the results of the simulations with the observed disc properties in sigma-Orionis, it will be possible to identify the evolutionary scenario that best reproduces the observations, characterizing how disc properties in sigma-Orionis are shaped by the environment, and inferring the initial conditions of the population of protoplanetary discs.

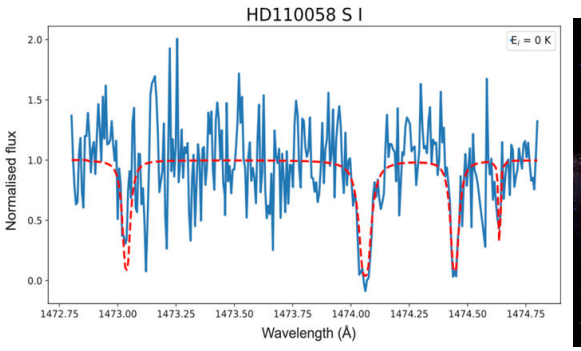
## Exploring the detectability of atomic sulfur emission released by young exocomets with the James Webb Space Telescope

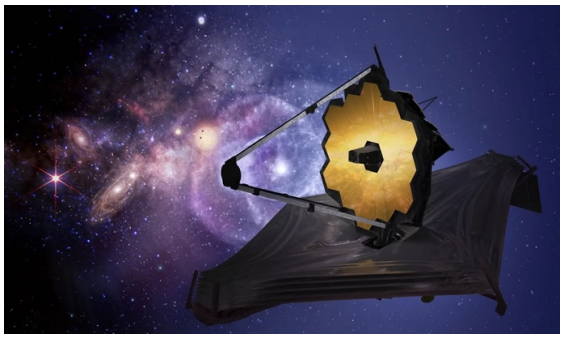
Prof. Luca Matrà
lmatra@tcd.ie

The majority of nearby, young (10s of million year-old) stars host bright disks/belts of icy exocomets akin to the Kuiper Belt in our Solar System, also known as *debris disks*. While these were previously thought to be gas-free, Atacama Large Millimeter/submillimeter Array (ALMA) observations now have the sensitivity to detect gas. The gas species detected with ALMA are carbon monoxide (CO) and neutral atomic carbon (C I); the former is likely released from ice on exocomets within the belt, with C I produced by CO photodissociation.

Surprisingly, neutral atomic sulfur gas (S I) was recently detected by the Hubble Space Telescope (HST) in absorption along the line of sight for edge-on disks (see spectrum below, Qi et al. in prep). This indicates that sulfur-bearing molecules must be present as well, although they are yet undetected. As absorption studies only probe the gas column along the line of sight to the star, emission studies sensitive to cold S I are now needed to establish 1) how much sulfur is present, and 2) whether it is co-located and also being produced in the exocometary belt at tens of au.
Sulfur is important because sulfur-bearing species play a role in origin-of-life chemistry (e.g. Patel et al. 2015), so establishing its presence on exocomets in the latest stages of terrestrial planet formation provides a route for their delivery to otherwise dry terrestrial planets like the Earth would have been in its infancy.

The project will focus on predicting the detectability of atomic sulfur (S I) emission with the mid-infrared MIRI/MRS instrument on the James Webb Space Telescope (JWST), through its $^3P_1$-$^3P_2$ spectral line at 25.25 $\mu$m. The project will involve largely Python coding, the JWST exposure time calculator, and potentially the 3D radiative transfer modelling tool RADMC-3D to model line emission and its detectability with JWST in systems where S I absorption is known to be present.



References:
- Patel et al. 2015, Nature Chemistry, https://www.nature.com/articles/nchem.2202
- Fitzsimmons et al. 2023, Comets III review chapter (Exocomets section), https://arxiv.org/abs/2303.17980
- JWST MIRI documentation (MRS specifically), https://jwst-docs.stsci.edu/jwst-mid-infrared-instrument

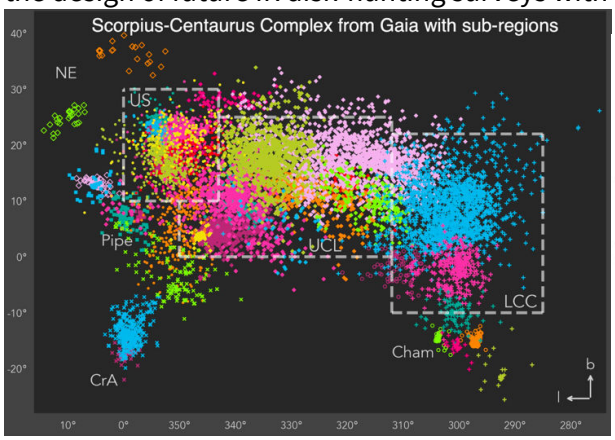
## Disk Hunting within the Scorpius-Centaurus Young Stellar Association

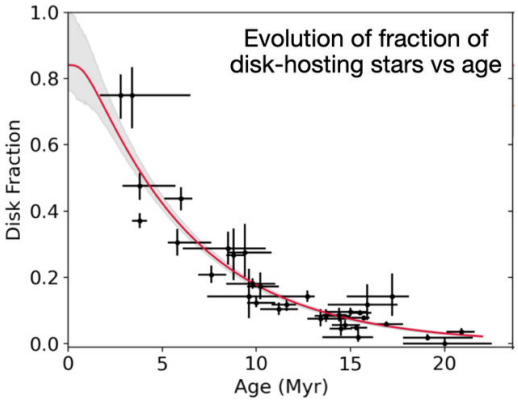
Prof. Luca Matrà - lmatra@tcd.ie

(Exo)Planets form in circumstellar disks of gas and dust, known as *protoplanetary* disks, around young stars. Here, dust from the interstellar medium grows to planets as seen in our Solar System and around other stars. Protoplanetary disks evolve over timescale of ~few/10 million years (Myr) to leave behind a largely formed planetary system with planets and a gas/dust-poor debris disk (analogous to the Solar System's Kuiper or Asteroid belt).

In order to identify disks in the first place, we observe young star-forming regions and complexes in our Galaxy, starting from the nearest ones within 150 parsec, such as the Scorpius-Centaurus (Sco-Cen) association, hosting young stars <1 to ~30 Myr in age. After identification of the stars belonging to these regions, which has been recently revolutionised by the *Gaia* mission at optical wavelengths, the hunt for circumstellar disks is on. Dust-bearing disks are found by detecting excess continuum flux compared to what is expected from a 'naked' star at IR wavelengths, where the cold dust can outshine the (hot) host star. Our entire knowledge of planet formation rests on this disk detection method.

The project will start from the tabulated Gaia-defined population of 1000s of star in Sco-Cen to re-evaluate the efficacy of excess-detection methods and inferences on disk evolution using existing mid-IR data from the WISE and (where available) *Spitzer* space telescopes. The immediate goals will be to 1) understand the limit of these disk-finding techniques, in other words evaluating the faintest disk disk flux detectable at various IR wavelengths, around different host stars in Sco-Cen, and 2) build the cumulative flux distribution of disks in the Sco-Cen at different IR wavelengths, comparing it amongst young stars of different masses and ages, in order to move forward from existing, simple 'disk fraction vs mass/age' analyses to a detailed 'disk brightness distribution vs mass/age' – all within the same environment of the Sco-Cen complex. Crucially, this project will inform the design of future IR disk-hunting surveys with the *James Webb* Space Telescope.




**References:**

- Williams & Cieza 2011, ARA&A review, https://arxiv.org/pdf/1103.0556
- Luhman et al. 2022a and b, AJ, https://ui.adsabs.harvard.edu/abs/2022AJ....163...24L/abstract and https://ui.adsabs.harvard.edu/abs/2022AJ....163...25L/abstract
- Ratzenbock et al. 2023, A&A, https://ui.adsabs.harvard.edu/abs/2023A%26A...678A..71R/abstract
- Polnitzky et al. 2026, A&A, https://ui.adsabs.harvard.edu/abs/2026A%26A...707A.216P/abstract

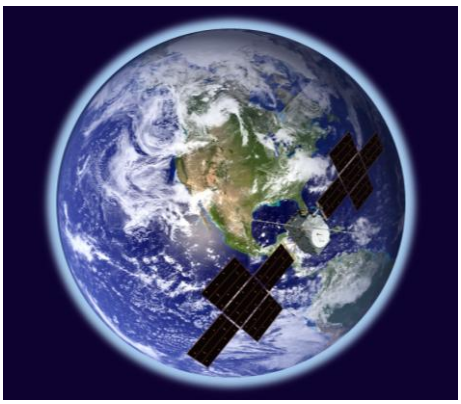
# Supporting the Jupiter Icy Moons Explorer: Analysis of different spacecraft observations of Earth's space environment

**Dr. Mika Holmberg and Maryam Zeroual**

mika.holmberg@dias.ie

**Research Project Description:**

The European space mission Jupiter Icy Moons Explorer (JUICE) was launched in April 2023 and will arrive at Jupiter in 2031. The mission's main objective is to study Jupiter and its space environment, with a particular focus on the potential habitability of its icy moons. As part of its journey to Jupiter, JUICE performed its first Earth gravity assist in August 2024. This maneuver gave us an excellent opportunity to collect scientific data about the Earth's near-space environment.



Impression of JUICE during the 2024 Earth swing-by. Earth image credit: NASA and JUICE image credit: ESA.

This project, divided in two parts, provides an opportunity to support the JUICE mission focusing on this period during the 2024 Earth gravity assist. Part 1 will look at cataloguing all relevant Earth space missions with the appropriate instrumentation. The trajectories of these currently active missions will then be visualised relative to JUICE. Part 2 will be to analyse the observations made by the NASA mission, the Van Allen probes. These results will be used to better understand the space environment here, which will then be used to improve the data analysis of the JUICE observations.

**References:**

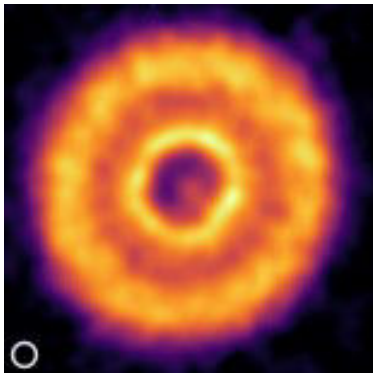
Below are some references to help you learn more. The first provides an overview of the magnetosphere around Earth, the region influenced by Earth's magnetic field. This can be read with the third reference which provides more detail about the specific region in the magnetosphere, the plasmasphere. The second reference gives an introduction to the Juice mission and its objectives, in particular sections 1, 2 and 3.1. The fourth is an example of our research giving an idea of the application of this work, and the final reference is particularly relevant for the second part of the project.

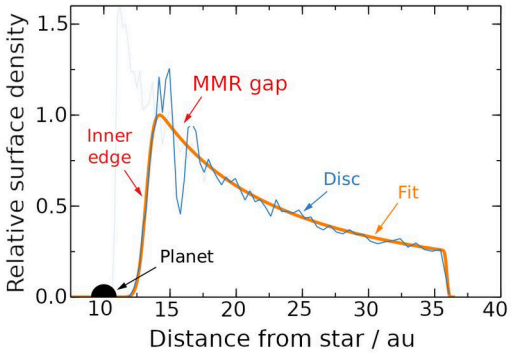
1. Borovsky, J.E. and Valdivia, J.A. (2018). The Earth's magnetosphere: A systems science overview and assessment. https://link.springer.com/article/10.1007/s10712-018-9487-x
2. Grasset, O., et al. (2013). JUpiter ICy moons Explorer (JUICE): An ESA mission to orbit Ganymede and to characterise the Jupiter system. https://www.sciencedirect.com/science/article/pii/S0032063312003777
3. Singh, A.K., Singh, R.P. and Siingh, D. (2011). State studies of Earth's plasmasphere: A review. https://www.sciencedirect.com/science/article/pii/S0032063311001000
4. Zeroual, M., et al. (2026). Surface charging of the JUICE spacecraft during the 2024 Earth gravity assist. https://egusphere.copernicus.org/preprints/2026/egusphere-2026-2068/
5. Rasinskaite, D., et al. (2025). Estimating electron temperature and density using Van Allen probe data: Typical behavior of energetic electrons in the inner magnetosphere. https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2024JA033443

# Planets carving gaps in cometary belts

**Prof. Tim Pearce, Trinity College Dublin** (email: tim.pearce@warwick.ac.uk)

'Debris discs' are belts of asteroids or comets orbiting stars, like the Asteroid Belt and Kuiper Belt in our Solar System. Many debris discs are imaged around other stars (left figure), and we think that almost all stars host such discs. For a first introduction to debris discs, see [1].






*Left: a debris disc imaged around another star [2]. The star is in the centre (not visible at this wavelength), and surrounded by a debris disc extending from 50 to 150 au. This disc has a gap. Right: theoretical profile of a different disc, from an n-body simulation of a planet interacting with a debris disc (blue). The fit (orange) works for the overall profile, but does not capture the MMR gap around 16 au.*

Debris discs show extraordinarily diverse features. Some contain gaps, like in the figure, which are unexplained. This project would help understand such gaps.

Planets can carve gaps in debris discs [3]. One way is through 'mean-motion resonances' (MMRs), which occur when bodies' orbital periods are simple fractions of each other. If debris and a planet are in MMR, then the debris gets excited, which carves a gap. MMR gaps are the focus of this project.

The widths and depths of MMR gaps, and their dependence on planet mass and orbit, have not been explored. This project takes existing *n*-body simulations of planets interacting with debris discs [4], and extracts disc profiles (right figure). Current fits to these profiles (orange line) fail to capture MMR structure (around 16 au on the figure). The project aims to empirically devise simple, general equations describing MMR gaps as functions of planet properties. These would be calibrated and tested against ~1000 *n*-body simulations of different planets and discs. The equations could be used by the community to predict MMR gaps from planets, and infer whether observed gaps could be carved by this mechanism. This project is mainly computational with some analytics, and requires Python experience.

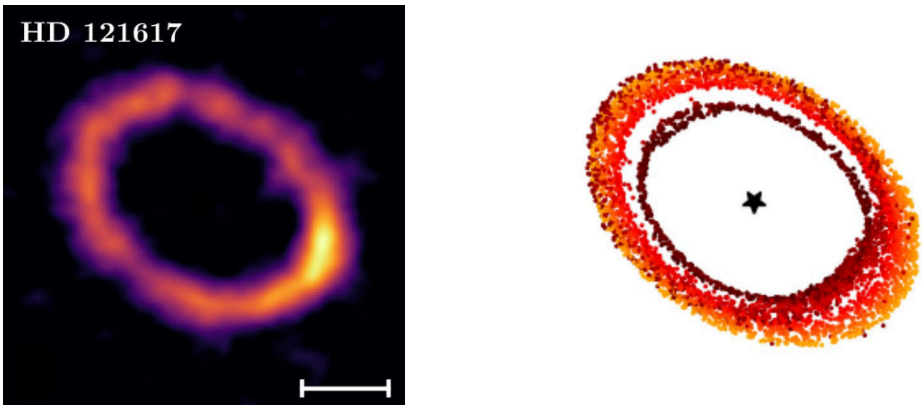
**References**

[1] Pearce 2026, *Encyclopedia of Astrophysics*, Volume 1, Elsevier, pp. 270-287
[2] Marino et al. 2018, MNRAS, 479, 5423
[3] Friebe et al. 2022, MNRAS, 512, 4441
[4] Pearce et al. 2024, MNRAS, 527, 3876

# Constraining an unseen planet from a clump in a cometary belt

**Prof. Tim Pearce, Trinity College Dublin** (email: tim.pearce@warwick.ac.uk)

'Debris discs' are belts of asteroids or comets orbiting stars, like the Asteroid Belt and Kuiper Belt in our Solar System. Many debris discs are imaged around other stars (left figure), and we think that almost all stars host such discs. For a first introduction to debris discs, see [1].




*Left: a debris disc imaged around the star HD 121617 [2]. The star is in the centre (not visible at this wavelength), and surrounded by a debris disc at ~80 au. This disc has a 'clump', visible as the bright feature on the right side. Right: an n-body simulation of disc structure arising from an interaction with a planet. The simulation produces a clump in the correct location, but is not a perfect match.*

The particular debris disc imaged around the star HD 121617, shown on the left image, contains a 'clump': an overdensity of material. The origin of this clump is unknown, but it is potentially due to interactions with a hypothetical planet orbiting interior to the disc. Simulations of such interactions in other systems can produce similar clumps [3].

The aim of this project is to use the observed clump in HD 121617 to constrain the mass, orbit and possible migration rate of a hypothetical planet in this famous system. This would be achieved through *n*-body simulations of planet-disc interactions, plus semi-analytic models. These simulations and models would be used to generate simulated images for comparison with observations, to find the family of planet parameters that can reproduce the data.

Some image-processing tools, semi-analytic models and *n*-body simulations already exist, but these will need modifying and expanding to allow a detailed parameter search. This project is mainly computational with some dynamical analytics, and requires Python experience. IDL experience would also be useful, but not necessary.

**References**

[1] Pearce 2026, *Encyclopedia of Astrophysics*, Volume 1, Elsevier, pp. 270-287
[2] Marino et al. 2026, A&A, 705, A195
[3] Booth et al. 2023, MNRAS, 521, 6180

# Lyman-α as a Probe of Ionizing Escape and the Intergalactic Medium

**Dr. Ryan Begley**
ryan.begley@armagh.ac.uk

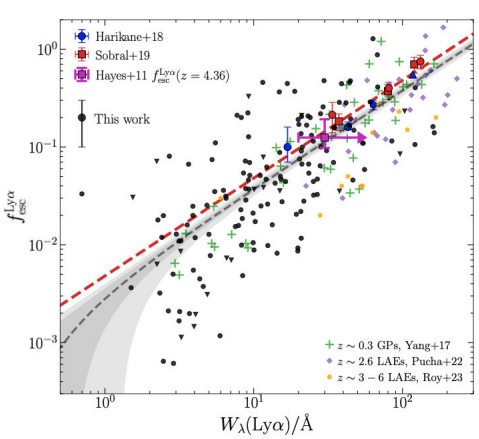
Note: this project can be run either in-person, hybrid or remotely to suit the circumstances of the student. Feel free to get in touch to discuss further if needed.

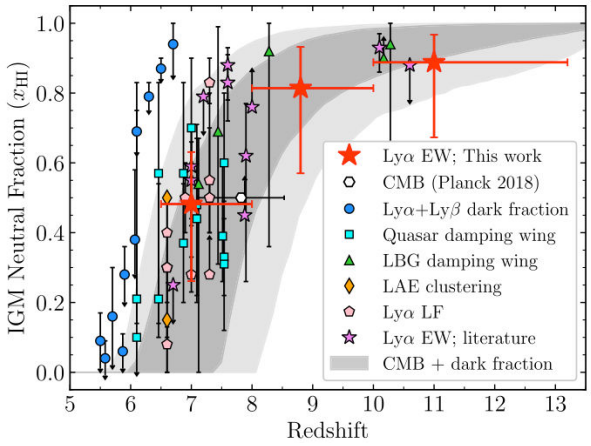
## Research Project Description:

The Lyman-alpha (Lyα) emission line is one of the most powerful observational probes of galaxies in the distant Universe. Because Lyα photons are resonantly scattered by neutral hydrogen, their escape from galaxies depends sensitively on the distribution of gas and dust within galaxies, as well as the ionization state of the surrounding intergalactic medium (IGM). As a result, Lyα provides a unique window into both the internal physics of galaxies and the large-scale evolution of the Universe during and after the epoch of reionization.

This project will investigate the physical drivers of Lyα emission in star-forming galaxies using spectroscopic datasets from surveys such as MUSE, with the option to incorporate complementary constraints from the James Webb Space Telescope where available. The student will move beyond simple classifications of Lyα emitters and instead explore how the strength and visibility of Lyα emission vary as a function of galaxy properties such as luminosity, UV colour, and redshift.

A key aim of the project will be to test whether Lyα emission can be predicted from observable galaxy properties, and to identify the dominant physical factors that regulate its escape. By quantifying these relationships, the student will assess the extent to which Lyα can be used as an indirect tracer of ionizing photon escape and as a probe of the evolving ionization state of the IGM. This project will contribute to our understanding of how radiation escapes from galaxies and how early galaxies interact with their environments, providing important insight into the processes that governed cosmic reionization.




Left: Lyα escape as a function of Lyα emission line strength (Begley et al. 2024)

Right: Evolution of the neutral Hydrogen fraction, tracing the Epoch of Reionization (Tang et al. 2024)

This project will provide the student with experience in analysing spectroscopic datasets from large astronomical surveys such as MUSE. They will learn how emission lines are measured and interpreted, and how spectroscopic observations are used to probe the physical properties of galaxies and the intergalactic medium.

The student will develop skills in handling and analysing scientific datasets using Python, including statistical analysis and data visualisation. They will also gain insight into how astronomers use observational data to infer physical processes such as gas distribution, dust attenuation, and the escape of radiation from galaxies.

## References:

Begley et al. 2024 - https://arxiv.org/abs/2306.03916
An analysis investigating how Lya can inform insights of the escape of ionizing radiation.
Tang et al. 2024 - https://arxiv.org/abs/2408.01507
Investigation of high-redshift LAEs using JWST, with implications for the evolution of the IGM
Kerutt et al. 2022 - https://arxiv.org/abs/2202.06642
Study of the connection between Lya and galaxy properties using MUSE.

# Machine Learning Representations of High-Redshift Galaxies

**Dr. Ryan Begley**
ryan.begley@armagh.ac.uk

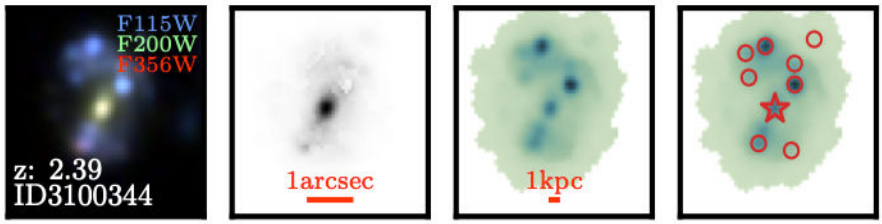
Note: this project can be run either in-person, hybrid or remotely to suit the circumstances of the student. Feel free to get in touch to discuss further if needed.

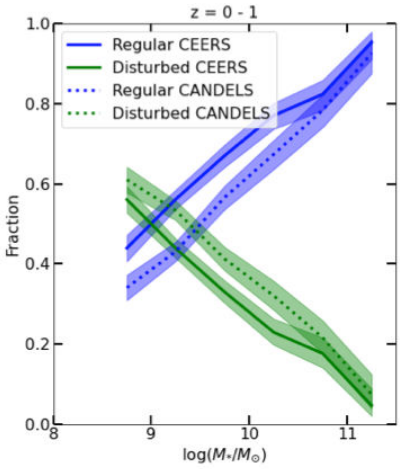
Research Project Description:

Deep imaging from the Hubble Space Telescope and the James Webb Space Telescope has revealed that galaxies in the early Universe exhibit a wide range of complex and often irregular structures. Interpreting these morphologies is challenging, as traditional approaches rely on simplified models or human classification, which do not scale well to modern datasets.

This project will apply self-supervised machine learning techniques to galaxy imaging to uncover underlying patterns in galaxy structure at high redshift. By training models to learn compact representations of galaxy images, the student will investigate whether these representations correlate with key physical properties such as redshift, stellar mass, and star formation rate.

The project will explore how galaxies are distributed within this learned "latent space", and assess whether it provides a useful framework for classification, clustering, and identifying unusual systems. This work will contribute to the development of new data-driven tools for studying galaxy evolution in the era of large astronomical surveys




Left: Example of a galaxy selected from CANUCS with a highly clumpy morphology (Sok et al. 2025)

Right: Fraction of "regular" & "disturbed" galaxies versus their stellar mass (Huertas-Company et al. 2024)

Throughout this project, the student will gain hands-on experience with JWST/NIRCam imaging from deep surveys and inferring morphological properties of galaxies. These observational datasets will then be combined with traditional statistical methods, as well as explore the use of machine learning to better connect galaxy properties with their morphology.

References:

Huertas-Company et al. 2024 - https://arxiv.org/abs/2305.02478
Explores redshift evolution of galaxy morphology using JWST imaging
Sok et al. 2025 - https://arxiv.org/abs/2509.25363
Investigates properties of star-forming clumps within galaxies from the JWST CANUCS survey.
Tohill et al. 2024 - https://arxiv.org/abs/2306.17225
Uses machine learning on JWST galaxy images to perform feature extraction, and connect with aspects of galaxy formation.

# Preparing for the Roman Space Telescope
*Photometric redshifts and galaxy populations*

**Dr. Ryan Begley**
ryan.begley@armagh.ac.uk

Note: this project can be run either in-person, hybrid or remotely to suit the circumstances of the student. Feel free to get in touch to discuss further if needed.

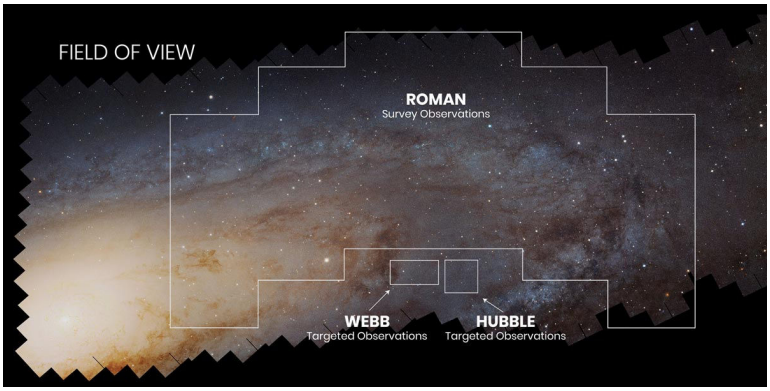
Research Project Description:

The upcoming Nancy Grace Roman Space Telescope will revolutionise wide-field infrared astronomy, providing deep imaging over areas far larger than current JWST surveys. Equipped with its Wide Field Instrument and an exceptionally large field of view, Roman will observe hundreds of millions of galaxies over its lifetime, producing data volumes vastly exceeding those of existing facilities. This shift into the "big data" era of astronomy presents both an opportunity and a challenge: new, scalable methods are required to efficiently extract physical information from these enormous datasets.

This project will explore how well galaxy distances (photometric redshifts) and key physical properties can be recovered from Roman-like data. Using simulated galaxy catalogues or mock observations, the student will investigate how observational uncertainties, such as limited wavelength coverage, photometric noise, and source blending, affect our ability to infer galaxy properties. Particular focus will be placed on understanding how these uncertainties propagate into measurements of galaxy populations, including luminosity functions, stellar mass distributions, and the inferred evolution of galaxies across cosmic time.

A key component of the project will be to assess how Roman's wide-area imaging can be combined with deeper, higher-resolution data from the James Webb Space Telescope. By exploring these synergies, the student will examine how small, detailed JWST samples can be used to calibrate and interpret the much larger statistical samples from Roman.

This project will provide insight into how future surveys will measure galaxy evolution on unprecedented scales, and will help develop the tools needed to fully exploit the next generation of astronomical datasets.




Field of view from a single image with Roman versus JWST and HST Credit: STScI

Throughout this project, the student will gain broad experience in observational imaging techniques, statistical modelling and using simulated galaxy data products. They will learn to measure galaxy properties, including implementing photometric redshift techniques and assessing the impact of observational uncertainties on population studies. The project will also introduce modern data-driven approaches, potentially including elements of machine learning, providing valuable preparation for research in the era of large astronomical surveys.

References:

Bagley et al. 2026 - https://arxiv.org/abs/2603.09828
An investigation of possible surveys to be carried out with Roman using the Santa Cruz SAM, with implications for the measured population statistics of high-redshift galaxies.
Khederlarian et al. 2026 - https://arxiv.org/abs/2602.10207
Demonstration for application of ML methods to infer photometric redshifts in Roman datasets.

# Spatially resolved star-formation in the high-redshift Universe with JWST

**Dr. Ryan Begley**
ryan.begley@armagh.ac.uk

Note: this project can be run either in-person, hybrid or remotely to suit the circumstances of the student. Feel free to get in touch to discuss further if needed.

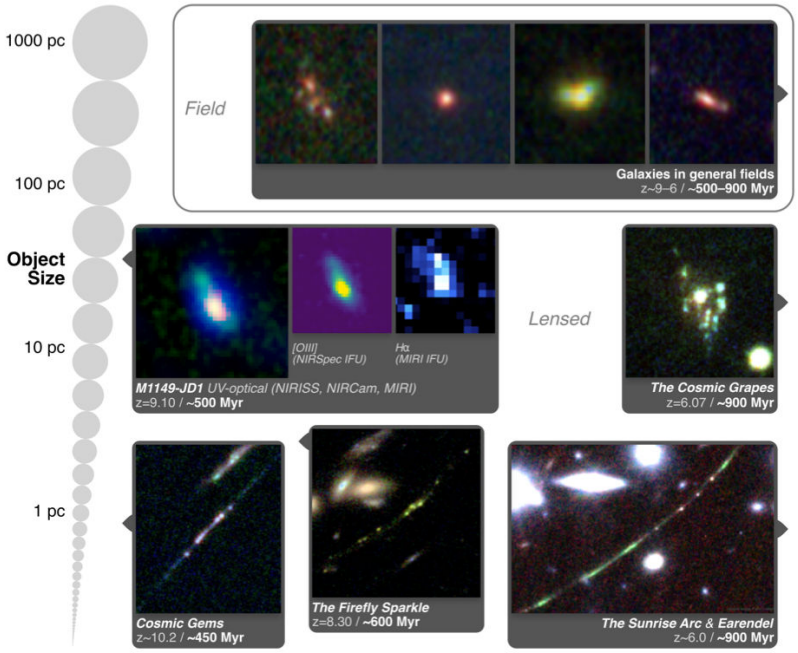
Research Project Description:

The latest observations from the James Webb Space Telescope have revealed that galaxies in the early Universe are not simple systems, but instead often exhibit clumpy, irregular structures. These features are thought to trace regions of intense star formation and may provide insight into how galaxies assemble their mass over time.

This project will investigate the spatially resolved structure of high-redshift galaxies by quantifying their morphologies and identifying clumpy or compact star-forming regions. Using high-resolution imaging, the student will measure structural properties such as galaxy size, concentration, and asymmetry, and develop simple metrics to quantify clumpiness.

The student will then explore how these structural properties correlate with global galaxy observables such as UV luminosity and colour, testing whether morphology can act as a predictor of galaxy physical state.

This project will provide insight into how star formation proceeds on sub-galactic scales in the early Universe, while introducing the student to modern techniques in galaxy morphology and imaging analysis.




Examples of resolved galaxy morphologies and clumpy star-formation in the high-redshift Universe (Adamo et al. 2024)

Throughout this project, the student will get hands-on experience with high-resolution imaging data from JWST, developing practical skills in astronomical image analysis, including galaxy morphology measurements. The student will gain experience in statistical modelling, and introduce key concepts in galaxy formation and evolution, including star formation at high-redshift.

References:

Adamo et al. 2024 - https://arxiv.org/abs/2405.21054
A review paper highlighting recent key results about galaxy evolution / formation in the first Gyr from JWST, including new insights based on spatially resolved analyses.
Giménez-Arteaga et al. 2022 - https://arxiv.org/abs/2212.08670
First demonstration of spatially resolved galaxy properties with JWST ERS data
Zhu et al. 2026 - https://arxiv.org/abs/2601.15965
Latest example of paper studying the properties of clumpy features within galaxies, and connecting these regions to physical processes.

# Resolving solar flares at the smallest scales with ESA's Solar Orbiter

**Supervisor:** Dr. Laura A. Hayes (laura.hayes@dias.ie)
**Host Institution:** Dublin Institute for Advanced Studies (DIAS)

**Research Project Description:**

Solar flares are sudden, powerful bursts of energy released on the Sun, driven by the rapid reconfiguration of magnetic fields in its atmosphere. In ultraviolet light, they appear as bright elongated features known as flare ribbons, which mark where energy is deposited into the lower solar atmosphere. Until recently, observations have been limited by instrument saturation and cadence, making it difficult to resolve the smallest and fastest-evolving structures within these ribbons. It is therefore unclear whether flare ribbons are smooth features or instead composed of many small, short-lived brightenings known as flare kernels.

ESA's Solar Orbiter mission now provides a new view of flares. Its Extreme Ultraviolet Imager (EUI) captures high-resolution, high-cadence images, and short-exposure observations avoid saturation during the brightest phases, revealing fine-scale structure that was previously hidden (see Fig 1). At the same time, the Spectrometer/Telescope for Imaging X-rays (STIX) measures X-ray emission from high-energy electrons, offering a complementary probe of energy release. These observations are often obtained during Solar Orbiter's Major Flare Campaigns, coordinated observing periods designed to capture flares at high cadence with multiple instruments (e.g. Ryan et al. 2025; Collier et al. 2026).

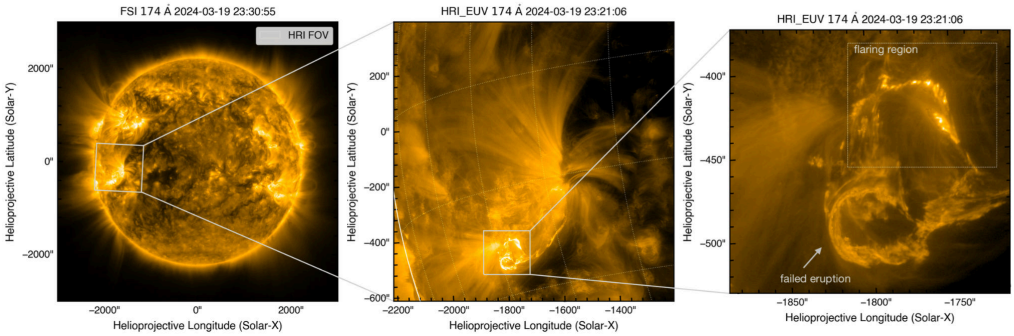



*Figure 1: Solar Orbiter/EUI observations of a flare caught during the major flare campaigns at the highest spatial and temporal resolution of a flare to date in the EUV.*

In this project, the student will analyse one or more solar flares observed during these campaigns, directly working with high-resolution spacecraft data to identify and track individual energy-release sites in the observations. The student will:

- Work with EUI image sequences and corresponding STIX X-ray lightcurves for a selected flare event observation
- Identify compact bright regions ("flare kernels") using in the EUI images using image processing techniques (e.g. thresholding or segmentation)
- Track their evolution through time by linking structures across successive images
- Measure properties such as size, lifetime, brightness, and motion along the ribbons
- Construct simple EUV intensity time series and compare these with STIX X-ray lightcurves to investigate the timing of energy release and plasma response

The project will be carried out in Python using community-developed tools (e.g. SunPy), providing experience in scientific programming, image analysis, and working with data from a current ESA space mission. The overall aim is to determine whether flare ribbons are composed of discrete, rapidly evolving energy-release sites and how these relate to the timing of particle acceleration in solar flares.

## Real-time Denoising of Scanning Transmission Electron Microscopy Images

Prof. Lewys Jones & Dr Jon Peters, Ultramicroscopy Research Group

(www.tcd.ie/Physics/research/groups/ultramicroscopy/)

**Keywords:**

Scanning transmission electron microscopy (STEM), low-dose imaging, image processing, GPU programming.

**Abstract:**

Electron microscopes use a beam of accelerated electrons as their illumination rather than visible light. As a result, they can achieve far greater magnifications and resolutions down to the atomic scale. The scanning transmission electron microscope (STEM) uses a focussed probe of electrons, that is rastered point by point.

When imaging fragile or radiation-sensitive samples, the lowest practical beam-current is used, but this leads to noisy images that are more difficult to reliably interpret. Denoising software can partially remediate this, but this is often done after the experiment is concluded.

At fast imaging rates, we might capture 20 frames-per-second or more. Viewing these images in real-time is essential for the operation of the microscope. However, the image denoising cannot run as fast as the recording. This project will continue earlier work in the group which developed a rapid image denoising code (Figure 1).

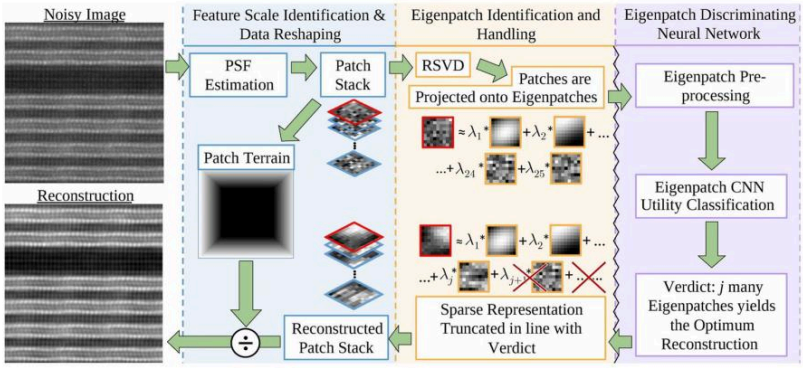



*Figure 1. Schematic of REUCID denoising workflow from noisy input to reconstructed output [1].*

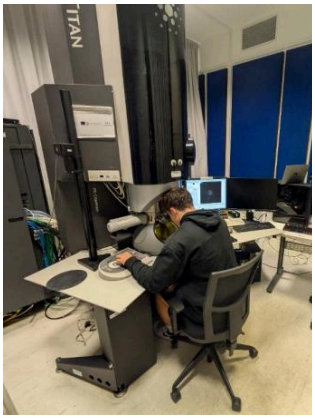


*Figure 2. Previous SS student using the 300kV Titan microscope.*

The goal is to accelerate the code (already written in Python by past PhD and SS students), using either parallelised CPU cores or high-performance GPUs available in the lab. This will then be deployed to run live at the electron microscope.

**Expected Outcomes:**

During this project, with the support of others in the research group, the student will:

- Become familiar with the existing Python code.
- Develop methods to accelerate the code, or to port it to GPU parallelisation.
- Test the code online at the microscope with a live stream of data.

If the code works as expected, we aim to write a research paper on it's use.

**Further Details:**

The project and desk will be based in the Advanced Microscopy Laboratory (www.tcd.ie/crann/aml). The ideal student will have an interest in programming, image analysis, and computing. Experience with Python is essential, preferably an advanced knowledge.

[1] Mitchell, M.A.J., Sanvito, S. & Jones, L. Rapid eigenpatch utility classifier for image denoising. *Sci Rep* **15**, 16626 (2025). https://doi.org/10.1038/s41598-025-96859-x.

# SS Project Proposal 2024

## Project 1: Characterisation of solid state electrochromic thin films for flexible smart window applications

Prof. David McCloskey

### Research Project Description:

Electrochromic systems exhibit a change of colour on applied external voltage. This can be used to create smart windows with adaptable optical and thermal properties which can significantly reduce energy use in residential or office buildings[1].

There are many organic and inorganic materials that can be used to display this effect but the most commonly used in industry are inorganic films of transition metal oxides with $WO_3$ and $NiO_x$ as the most developed[2]. In an electrochromic cell there will be a working electrode, an electrolyte (usually liquid or polymer), an ion donor layer and a counter electrode. Under applied bias ions from the donor layer move through the electrolyte and are embedded in the electrochromic layer which changes its electronic and optical properties significantly. In general, the effect is due to an oxidisation /reduction cycle and can be seen as similar or charging/ discharging a battery. Energy is only required during switching and a good electrochromic material will retain its state for a long time after charging. In the application of smart windows for example, when the layer is uncharged it is transparent and when charged it becomes opaque. This allows for a very low energy technique to control the solar gain into the building which can significantly reduce air conditioning costs in the Summer and heating costs in Winter. Recent work has demonstrated structural colour tuning of electrochromic materials using thin film interference in Fabry Perot type geometries[3]. Since we have recently commissioned a new magnetron sputtering system we would like to investigate this effect further using our deposition system.

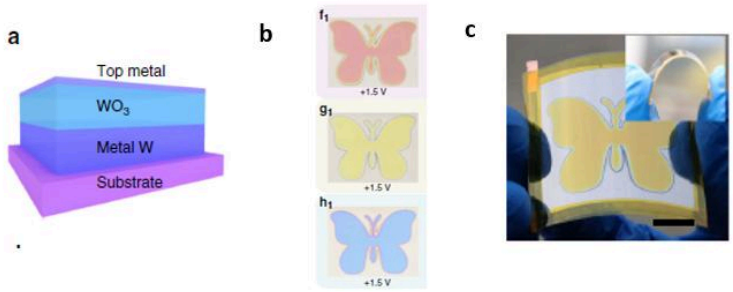



**Figure.1** (Adapted from Ref 3): **(a)** Metal insulator metal structure active electrode. **(b)** Example of colour change under applied external Bias **(c)** demonstration of deposition on flexible substrate.

### Project objectives

The student will be required to:

- Prepare a review of the literature on state-of-the-art electrochromic flexible window coatings.
- Design thin film layered structures for electrochromic thin films.
- Deposit thin films using Magnetron sputtering
- Tune properties using electrochemistry.

# SS Project Proposal 2026

**Real-World Coefficient of Performance (COP) of Domestic Heat Pumps in the Irish Climate: Economic and Policy Implications of the SEAI Grant System**

Heat pumps are central to Ireland's strategy for decarbonising residential heating under the Sustainable Energy Authority of Ireland (SEAI) and the national Climate Action Plan. Through capital grants and retrofit schemes, SEAI has incentivised widespread adoption of air-to-water and ground-source heat pumps in Irish homes. While manufacturer-reported Coefficient of Performance (COP) values are typically derived under standard laboratory conditions, there is growing evidence that real-world performance can vary significantly due to climate, installation quality, dwelling characteristics, and user behaviour. Ireland's mild but humid maritime climate presents unique operational conditions for heat pumps, including frequent defrost cycles and seasonal variability. Understanding the real-world COP under Irish conditions is critical for evaluating carbon savings, household energy costs, and the cost-effectiveness of public subsidy schemes. This project will investigate measured seasonal and annual COP values from operational domestic heat pump systems in Ireland and assess the economic and policy implications of the current grant framework.

The primary objectives of this MSc project are:

1. **Quantify Real-World Performance:** Collect and analyse monitored performance data (electricity consumption and heat output) from a representative sample of domestic heat pump installations in Ireland to determine seasonal performance factors (SPF) and annual COP values.
2. **Assess Climatic Influence:** Examine the relationship between outdoor temperature, humidity, and system performance to evaluate how Irish climatic conditions influence operational efficiency.
3. **Evaluate Economic Impacts:** Compare real-world running costs with projected costs based on design assumptions. Conduct a lifecycle cost analysis incorporating capital costs, SEAI grant support, electricity tariffs, and maintenance costs.
4. **Analyse Policy Effectiveness:** Assess whether current SEAI grant levels align with actual performance outcomes and carbon savings. Identify potential policy refinements to improve cost-effectiveness and equity of the grant system.
5.

**Methodology:** The project will use a mixed-methods approach:

- Collection of monitored system data from participating households or secondary datasets where available.
- Statistical analysis of COP/SPF across seasons and dwelling types.
- Comparison of measured performance with manufacturer specifications and design-stage estimates.
- Economic modelling of payback periods and net present value under different electricity price and grant scenarios. Marginal abatement study generating McKinsey Cost Curve.
- Policy analysis informed by performance findings and stakeholder interviews (if feasible).

**Expected Outcomes:** This research will provide robust, data-driven insights into the intersection of technical performance, economic viability, and public policy. By grounding analysis in real-world operational data, the study aims to support more effective deployment of low-carbon heating technologies in Ireland's transition to a sustainable energy future.

**References:** Hoyne, Seamus; O'Reilly, Padraic; and O'Shea, Michael (2020) "Optimisation of Air Source Heat Pumps in Residential Retrofits," *SDAR* Journal of Sustainable Design & Applied Research*: Vol. 8: Iss. 1, Article 3.doi:ttps://doi.org/10.21427/zaxs-ns88

**Project Proposal**

**Project title:**

Automated Exploration and Mechanistic Analysis of Xylobiose and Xylotriose Pyrolysis Reaction Networks

**Supervisor(s):**

Dr Bernardo Ballotta

**Senior Supervisor(s):**

Prof Stephen Dooley

**School:**

School of Physics, the University of Dublin, Trinity College Dublin, Dublin, Ireland

**Project Description**

The thermochemical conversion of lignocellulosic biomass into renewable fuels and chemicals is a key challenge in the transition toward sustainable energy systems. Hemicellulose derived sugars and oligomers, including xylobiose and xylotriose, are important intermediates formed during biomass pyrolysis and play a significant role in determining product distributions, gas formation, and char production [1]. Despite extensive experimental and modelling efforts, the detailed reaction mechanisms governing the thermal decomposition of these species remain poorly understood due to the complexity of the underlying reaction networks.

Recent advances in computational chemistry and automated reaction discovery now make it possible to investigate highly complex pyrolysis systems in a more systematic and less biased way. In particular, automated mechanism generation approaches can identify large numbers of competing reaction pathways that may be difficult to predict using intuition driven methods alone. This project will investigate the decomposition chemistry of xylobiose and xylotriose using automated reaction mechanism discovery and quantum chemical calculations.

The project will build on previous work on β-D-xylopyranose pyrolysis and extend these methodologies toward larger hemicellulose model compounds. Automated reaction exploration will be performed using AutoMeKin [2], which combines reactive molecular dynamics simulations, graph theory analysis, transition state identification, and quantum chemical optimisation of stationary points. Density functional theory calculations will then be used to refine key reaction pathways and evaluate their energetic feasibility.

The project may also include comparison of predicted products with available experimental pyrolysis data and discussion of implications for kinetic model development. Depending on the direction of the work, the student may focus more strongly on automated reaction discovery, quantum chemical calculations, reaction pathway analysis, or kinetic interpretation.

The broader impact of this work lies in improving the mechanistic understanding of biomass pyrolysis at the molecular level. Developing more reliable pyrolysis reaction networks for hemicellulose derived species can contribute to improved predictive kinetic models for renewable fuel production, bio-oil upgrading, and sustainable aviation fuel development. The project also provides experience in modern computational chemistry techniques increasingly used in chemical kinetics, catalysis, and energy research.

**References**

[1] Zhou, X., Li, W., Mabon, R., Broadbelt, L.J., A mechanistic model of fast pyrolysis of hemicellulose, Energy Environ. Sci. 11(5), 1240-1260 (2018).

[2] Martínez-Núñez, E., Barnes, G.L., Glowacki, D.R., et al., AutoMeKin2021: An opensource program for automated reaction discovery, J. Comput. Chem. 42(28), 2036-2048 (2021).

**Project title:** Molecular Physics Internal Energy Parameters in Multiphysics Models of CO2 Electrolysis Cells: Machine Learned Physics Evaluations
**Senior Supervisor(s):** Prof Stephen Dooley
**Project Description**
The electrochemical reduction of CO2 is widely recognized as a promising strategy for mitigating atmospheric CO2 while enabling the production of value-added chemicals and fuels. In recent years, substantial experimental and computational efforts have advanced both reactor performance and mechanistic understanding. In parallel, multidimensional multiphysics models, often referred to as digital twins, have emerged as key tools for describing electrochemical CO2 reduction systems and guiding reactor design. However, the predictive capability of these models critically depends on the accuracy and physical meaning of the kinetic and thermodynamic parameters used as inputs.

In practice, Multiphysics simulations frequently fail to quantitatively reproduce experimental observations or to provide reliable estimates of key physical quantities. A central limitation lies in the poor definition and large uncertainty of kinetic parameters governing both homogeneous electrolyte reactions and heterogeneous electrode processes. This project presents a comprehensive and systematic assessment of the kinetic and thermodynamic parameters employed in multiphysics models of CO2 electrolysis. The analysis is restricted to networks currently implemented in continuum simulations, comprising a minimal set of ~12 homogeneous electrolyte reactions coupled with lumped electrochemical pathways for CO2RR,
HER, and OER. By compiling and critically evaluating literature data, the variability of key parameters across studies is quantified, revealing that nominally identical molecular quantities can span multiple orders of magnitude and exhibit substantial sensitivity to experimental conditions and fitting methodologies.

This project provides a quantitative analysis of the number, type, and reliability of elementary processes represented in current multiphysics models, highlighting critical inconsistencies in parameter definition and transferability. The results will underscore that widely used molecular inputs should be interpreted as effective, condition-dependent descriptors rather than intrinsic constants, and emphasize the need for more rigorous, physics-informed data intensive parameterization strategies to enable predictive modelling of ECO2R systems.

**Keywords**— CO2 Reduction Cells, Multiphysics Simulations, Molecular Physics, Internal Energy, Kinetics, Data Science, Machine Learning.

The project ill include collection and data interrogation of molecular physics parameters required to solve CO2 electrochemical reduction by physical theories, including, heat capacity, ionization potential, collisional integral, rotational energy, vibrational energy, reaction rate constant, equilibrium constant.

[1] Sensitivity Analysis of One-Dimensional Multiphysics Simulation of $CO_2$ Electrolysis Cell
H Dunne, W Liu, MR Ghaani, K McKelvey, S Dooley
The Journal of Physical Chemistry C 128 (27), 11131-11144

[2] $CO_2$ Loss into Solution: An Experimental Investigation of $CO_2$ Electrolysis with a Membrane Electrode Assembly Cell
W Liu, H Dunne, B Ballotta, AA Massie, MR Ghaani, K McKelvey, ...
ACS Applied Energy Materials 7 (18), 7712-7723

**Zero-Moment Half-Metallic Ferrimagnets for use in Spintronic Frequency Multipliers - Stamenov (Experiment)**

The project will involve the experimental investigation of a relatively new class of magnetic materials – the Zero-Moment Half-Metals (ZMHM), using their prototype $Mn_{2-x}Ru_xGa$ (or MRG for short), in a thin film form. ZMHMs offer the rather unique for spin electronics combination of high bulk spin polarisation, stray field immunity and intrinsically high resonance and switching frequencies (in the low THz range). Nano-scale memory elements and terahertz oscillators, parametric frequency multipliers are only three examples of possible applications. Highly oriented and/or epitaxial films prepared by sputtering at different conditions (temperature, Ru-target current, etc.) will be used to conduct experiments on parametric excitation at high power levels in the microwave region. The measurements [magneto-transport, magnetometry and ferromagnetic resonance (FMR)] will be executed at both low-temperature and room-temperature, in magnetic fields of up to 14 T, in order to discern the influence of the two ferrimagnetic sub-lattices. The FMR measurements will be conducted with a field applied opposite to the remnant polarisation, in order to lower the resonance frequency to X-band microwaves. The 4$^{th}$ order in-plane anisotropy can give rise to parametric multiplication, generating modulation of the *z*-axis projection of the conduction electrons' spins at 4 times the source frequency. This can be detected by the corresponding modulation of the Hall conductivity of the sample, which in turn can produce the output signal and propagate it down a microwave waveguide. The information gained will be critical for the development of prototype magnetic devices working in the high-GHz and low-THz regions.

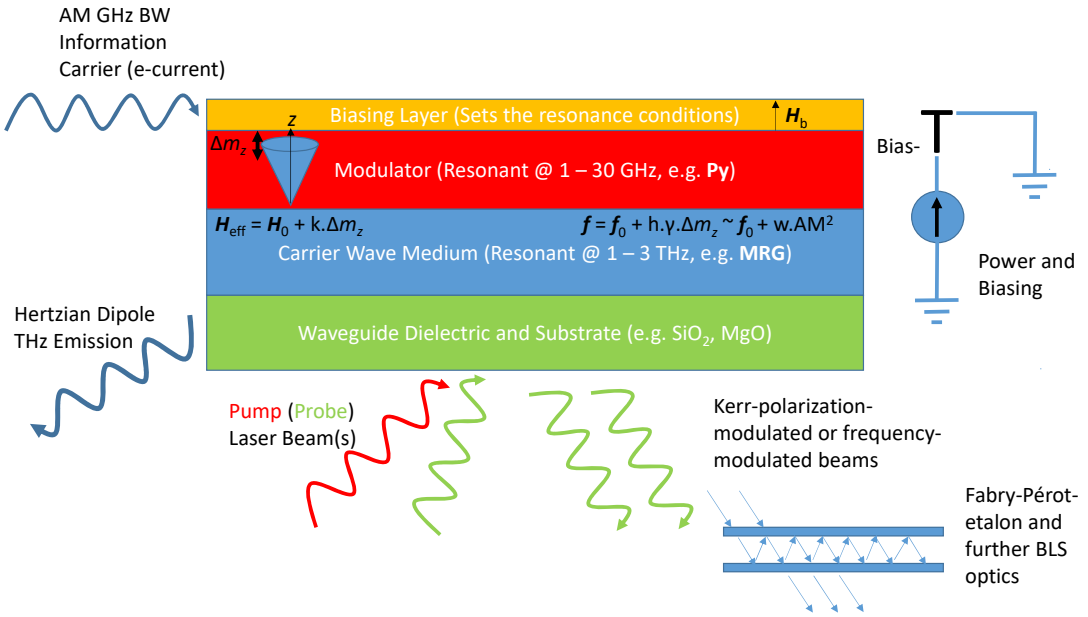



Fig. 1. A test structure utilizing the prototypical Zero-Moment Half-Metal $Mn_2RuGa$ (MRG), with its combination of 2-fold perpendicular and 4-fold in-plane anisotropy, and a conventional soft ferromagnet (i.e. permalloy), for the cross-modulation of signals between microwave bands in the 1 – 10 GHz region and ones above 40 GHz.

**Magnetically-Reconfigurable Diffraction Gratings Constructed of Amorphous Rare-Earth/Transition Metal alloys, for use in Beam-Steering and Magnetic Probabilistic Bit Arrays – Stamenov (Experiment)**

Magnetic materials are not new to data recording, with the high-capacity storage industry still relying heavily on magnetic hard drives and magnetic tape. There is one consumer storage format that has been, for a period, commercially successful – the MiniDisc™ [1]. Now essentially obsolete, it relies on a magnetic film of a rare-earth transition metal alloy (TbCoFe) that is re-written by means of heating it locally in a bias magnetic field (provided by a macroscopic magnet), using a focused laser beam. The readout takes advantage of the large magneto-optical Kerr effect exhibited by these materials. On the figure below there is an illustration of a MiniDisc in its protective cover and the structure of the media.

More recently, amorphous $DyCo_3$ and $TbCo_3$ alloys have attracted attention as of the possibility to do single-pulse (from an ultra-fast infrared fs-laser) magnetisation re-switching (toggling) in the absence of external magnetic field [2]. The process is partially deterministic and partially stochastic and could open possibilities for the realisation of optically-addressable probabilistic bit (p-bit) memory and logic, operating in the GHz region.

Following from successful work on the magnetic control of diffracted beams using commercial MiniDisc media, the aim will be to follow-up with diffraction gratings, deposited using the *Shamrock* and *Trifolium Dubium* deposition systems and characterised within the photonics laboratory, both located in the CRANN institute.

**References**

[1] https://en.wikipedia.org/wiki/MiniDisc.

[2] Zexiang Hu, et al. Single-pulse all-optical partial switching in amorphous $Dy_xCo_{1-x}$ and $Tb_xCo_{1-x}$ with random anisotropy, Appl. Phys. Lett. **120**, 112401 (2022).

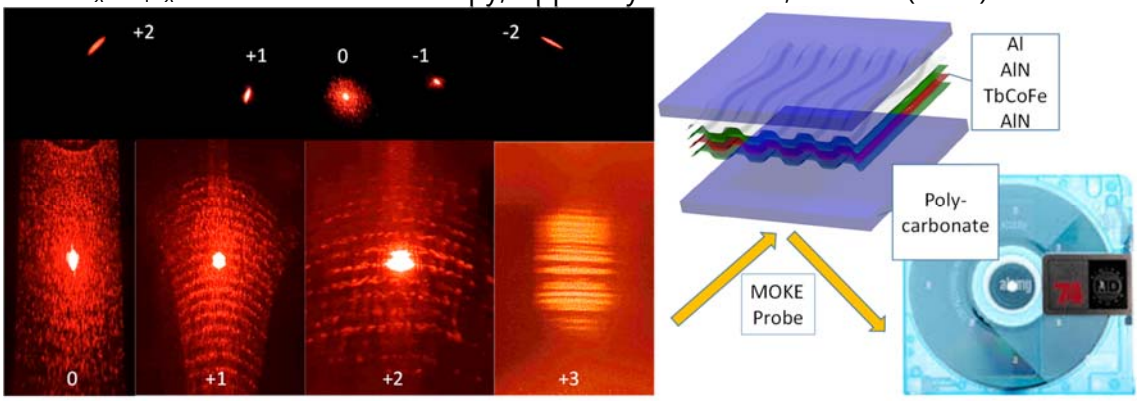



Figure: Experimental diffraction pattern (left) of the magnetic diffraction grating structure (middle) of a MiniDisk surface (right), showing the different diffraction modes and the superstructure related to the physical grooves within the protected reflective surface. The state of the diffraction grating can be altered via the application of magnetic field or via heating the magnetic material (e. g. using focused laser light).

## Geometrically-Optimized and Shared Memory (GPU)-Parallelized Elliptic Integrals Calculation for Magnetic Field Simulations and Metrological Coil Design - Stamenov (Theory/Computation/Experiment)

Modern computer hardware allows for unprecedented access to parallel computing, via the use of mixed CPU-GPU strategies, making good use of relatively inexpensive consumer grade hardware. Shared-memory parallel computing allows for speed/performance gains of orders of magnitude, in both general linear algebra calculations, and the evaluation of special functions. Despite the worsening double precision arithmetic (FP64) hardware performance of modern graphics cards, the sheer number of compute units often still dominates the limits of scaling and allows for the tackling of scientific calculation and engineering optimisation problems within comfortable time limits.

Here we propose to build upon existing work on the symmetry-geometrical optimisation of calculations heavily dependent on the evaluation of elliptic integrals of the first and second kind, such as calculation of the 3d-magnetic field profiles of metrological coils, electron microscopy magnetic lens and functional permanent magnet assemblies. The goal is to compute (including uncertainty budget), optimize and potentially prototype a new type of metrological source coil for weak magnetic fields (induction of < 10 mT), with homogeneity requirements at the few ppm levels. The work can involve a rough prototype of a geometry – optimized coil, or can remain purely theoretical/computational.

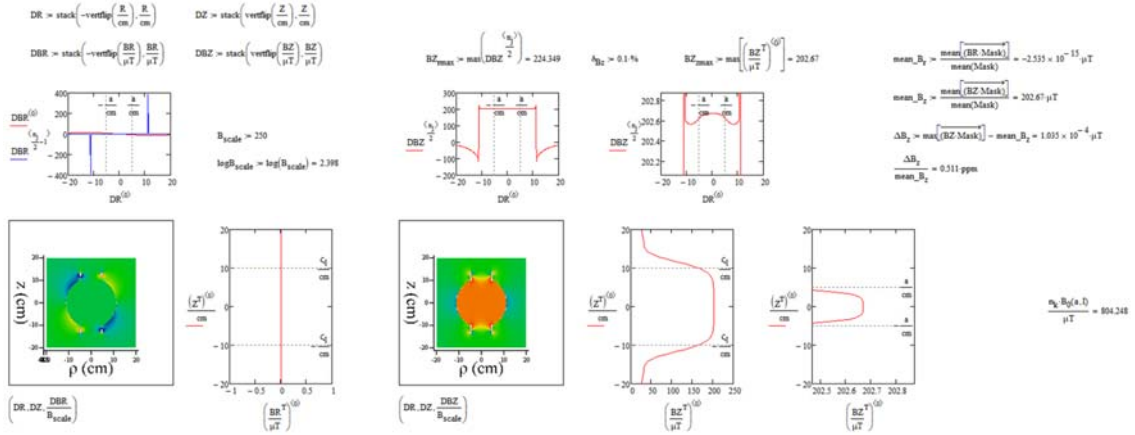



Fig. 1. A proposed, manually-optimized design of a quasi-spherical ultra-homogenous magnetic field metrological coil, dubbed 'Stamenov's bottle'. Homogeneity can reach below 0.5 ppm in a 1 cm diameter spherical volume in the middle of the assembly.

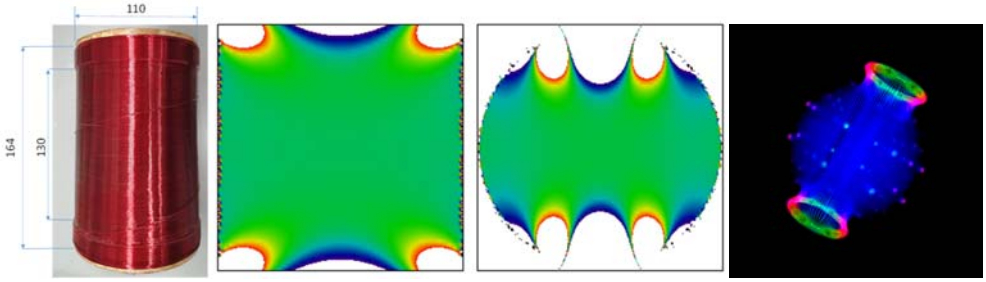



Fig. 2. Left-to-right: A picture of a calibration coil, its relative field profile shape, the relative field profile shape, and a volume rendering of the field, of the manually-optimized 'Stamenov's bottle'.

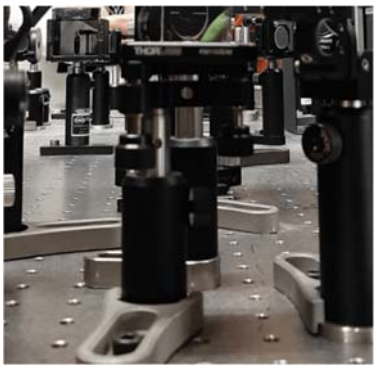
**Bulk Acoustic Wave (phonon) Coupling of Spintronic $Mn_2Ru_xGa$ Layers Through Thin Non-magnetic Membranes - Stamenov (Experiment)**

Project co-supervisor: Dr. Karsten Rode

In this project, we will explore experimentally the possibilities for the coupling of magnetic and lattice degrees of freedom in the prototypical compensated half-metallic $Mn_2Ru_xGa$ (MRG), a state-of-the-art material, developed in TCD for spintronic applications [1, 2].

Having explored previously very high frequencies (> 250 GHz) demagnetisation dynamics [3] and the nature of the magnetisation reversal and pinning [4] in MRG, here we want to elucidate the nature of magnon-phonon coupling in this unique material, combining high spin polarisation with low net magnetic moment and high magnetic resonance frequencies. The experiments to be conducted will include the growth of MRG on thin SiN membranes, with MgO buffering and their interrogation using ultrafast pulsed laser driven pump-probe stroboscopic experiments in the photonics laboratory of CRANN.

A variation of the measurement system used in [3] will be utilized, where the pump and probe laser beams can be directed at the opposing sides of the thin membrane carrying the sample magnetic layers. As the coupling between the two layers cannot be magnetic (net moment is rather small), bulk thermal waves and bulk acoustic waves ($k$ ~ 0 phonons) are left as the possible coupling mechanisms. These excitations have different characteristic group velocities and can be separated in the temporal domain.



Alternative ways of ultra-fast spin manipulation are essential for the development of new data processing and computing technologies.

The student involved will obtain solid understanding of the materials and their deposition, and experience in the operation of experimental setups involving ultrafast lasers.

[1] Giant spontaneous Hall effect in zero-moment $Mn_2Ru_xGa$, Naganivetha Thiyagarajah, Appl. Phys. Lett. **106**, 122402 (2015);
[2] Tunnelling magnetoresistance of the half-metallic compensated ferrimagnet $Mn_2Ru_xGa$, Appl. Phys., k. Borisov et al. Lett. **108**, 192407 (2016)
[3] Single pulse all-optical toggle switching of magnetization without gadolinium in the ferrimagnet $Mn_2Ru_xGa$, C Banerjee et al. Nature Communications volume **11**, 4444 (2020)
[4] Magnetic reversal and pinning in a perpendicular zero-moment half-metal, N. Teichert et al, Phys. Rev. Materials **5**, 034408(2021)

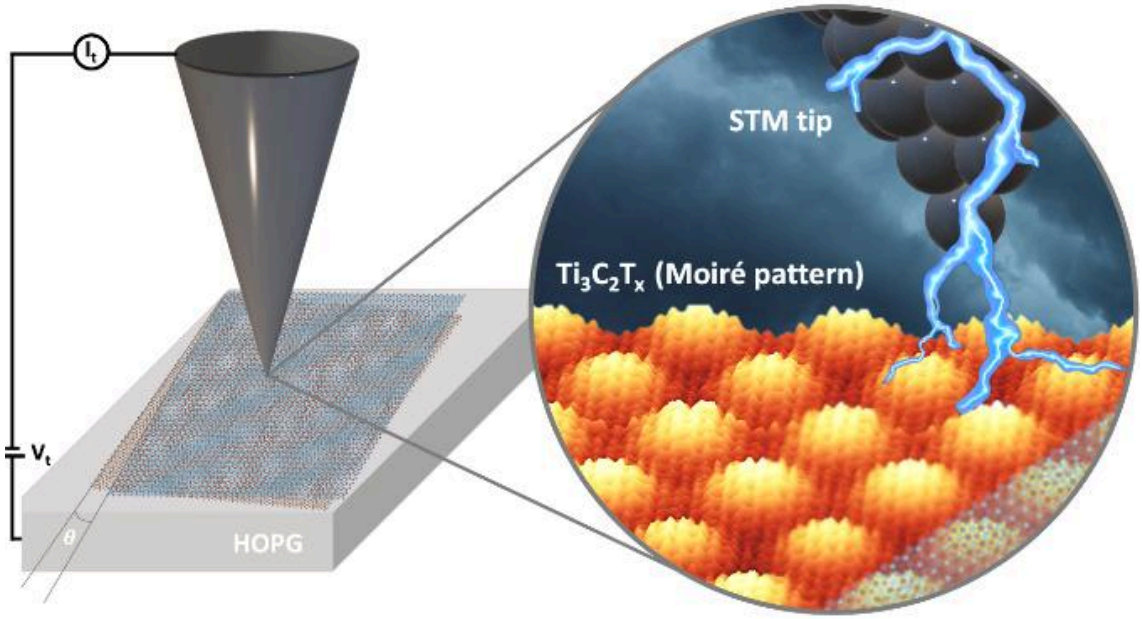
# Atomic-Scale Investigation of Moiré Superlattices in Liquid-Exfoliated 2D Materials

**Supervisor: Asst. Prof. Kuanysh Zhussupbekov**
**Email: kzhussup@tcd.ie**

Two-dimensional (2D) materials assembled into stacked or overlapping configurations can form Moiré superlattices, arising from lattice mismatch or rotational misalignment between adjacent layers. These superlattices introduce a long-wavelength periodic potential that can significantly modify the electronic structure, enabling emergent quantum phenomena such as correlated electronic states and band flattening [1], as well as tunable charge localisation [2], and the formation of strongly interacting electronic states in Moiré potentials [3]. Recent work on MXenes has demonstrated that self-assembled Moiré superlattices [4] can be formed through liquid-based processing routes, with periodicities on the nanometre scale and clear signatures of spatial modulation in the local density of states (LDOS), driven by interlayer coupling. However, the formation, control, and electronic consequences of such Moiré patterns in liquid-exfoliated 2D materials remain largely unexplored. This project aims to investigate Moiré superlattices formed in liquid-exfoliated 2D materials, including transition metal dichalcogenides (TMDs), MXenes, and related van der Waals systems. By exploiting the natural restacking and rotational disorder introduced during solution processing, the project will explore how twist angle, stacking configuration, and interlayer coupling influence electronic properties at the atomic scale.

**Objectives**

- To identify and characterise self-assembled Moiré patterns in liquid-exfoliated 2D materials
- To determine the relationship between twist angle and Moiré periodicity
- To investigate spatial modulation of the electronic structure (LDOS) induced by Moiré superlattices
- To explore how interlayer coupling and symmetry breaking modify band structure and electronic states
- To assess the potential of solution-processed 2D materials for twistronics applications




**References**

[1] Y. Cao *et al.*, "Unconventional superconductivity in magic-angle graphene superlattices," *Nature* **556** (2018), 43–50.
[2] C. R. Dean *et al.*, "Hofstadter's butterfly and the fractal quantum Hall effect in moiré superlattices," *Nature* **497** (2013), 598–602.
[3] Y. Jiang *et al.*, "Charge order and broken rotational symmetry in magic-angle twisted bilayer graphene," *Nature* **573** (2019), 91–95.
[4] K. Zhussupbekov *et al.*, "Self-Assembled Moiré Superlattices of $Ti_3C_2T_x$ MXene for Future Twistronic Applications," *Advanced Science* **12** (2025), e04394.

**Capstone Project - September 2026**

Jonathan Coleman

**Title**: Boosting electrical and optical performance of printed 2D materials by doping

Two-dimensional (2D) materials are emerging candidates for next-generation printed electronics due to their promising electronic and optoelectronic properties. Our group has developed methods to make electronic devices from 2D material inks, such as $MoS_2$, $WSe_2$ and InSe. Nevertheless, the absence of effective doping methods fundamentally results in energy barriers and high contact resistances at metal–semiconductor interfaces and thus restrict their practical applications. Doping is difficult because it often disturbs a homogeneous film formation and surface adsorbates strongly influence the charge carrier density and mobility. In this capstone project, a controlled doping method for $MoS_2$ and $WSe_2$ is developed to address this critical issue.

The project will begin by comparing the electrical and optical properties of printed $MoS_2$ and $WSe_2$ films with varying ionic liquid-based doping. The project provides a direct insight into the energy barriers using temperature-dependent sheet resistance. Using the most promising ionic liquid parameters, the project will next explore the device performance of doped $MoS_2$ and $WSe_2$ in thin film transistors.

The student will develop skills in solution-processing and printing of 2D materials, electrical characterization (sheet resistance, 2-probe current-voltage measurements, impedance spectroscopy), optical characterization (UV-Vis spectroscopy, optical microscopy). Furthermore, the student will have opportunities to observe more advanced materials characterization techniques such atomic force microscopy, photoluminescence spectroscopy and handling of cryogenics for temperature-dependent sheet resistance (liquid nitrogen). Furthermore, this Capstone project will support the student with highly relevant skills in data analysis, modelling and visualization.

Capstone Project - September 2026

Jonathan Coleman

Title: Electrical and mechanical properties of pressure-treated free-standing thin films of 2D nanosheets

Two-dimensional (2D) materials are poised to revolutionize nanotechnology owing to their unique electronic, optical, and optoelectronic properties that emerge at the nanoscale. Recently our group has developed a method to make free-standing films made up of entirely electrochemically exfoliated nanosheets without any additives. These thin films can be reduced to less than 100 nm in thickness while still being robust. A promising application is the assembly of individual film building blocks into heterostacks for flexible, thin devices. However, pressure is often needed to compress these films and keep them together, and little is known about the effects of pressure on the mechanical and electrical properties of the films, nor what range of forces can be applied to ensure the heterostacks remain together without damaging the individual films. This capstone project will systematically explore the effects of pressure on the mechanical and electrical properties of free-standing nanosheet films.

The project will begin by comparing the mechanical and electrical properties of free-standing graphene nanosheet films as a function of pressure, including max pressure and duration for a range of film thicknesses. Using the most promising parameters, the project will next explore the effect of the nanosheets themselves, comparing results for nanosheets of differing lengths and aspect ratio. Finally, the project will explore compressing stacks of films of same (homojunction) and different (heterojunction) materials to optimize material adhesion and performance across different materials and combinations.

The student will develop skills in mechanical characterization (tensile testing), electrical characterization (sheet resistance, 2-probe current-voltage measurements, impedance spectroscopy), and optical characterization (UV-Vis spectroscopy, optical microscopy). They will also learn about solution-phase production and processing of 2D materials. Furthermore, the student will have opportunities to observe more advanced materials characterization techniques such as scanning electron microscopy, atomic force microscopy, and photoluminescence spectroscopy.

**Capstone Project - September 2026**

Jonathan Coleman

**Title:** Solution-processed photodetectors based on chemically treated 2D semiconducting nanosheet networks

Two-dimensional materials (2DMs), due to their superb electronic and optical properties, are regarded as the next generation materials for (opto-) electronics. Recent advances in electrochemical exfoliation demonstrates that such nanosheets with atomically thin and large basal plane area could be obtained if an external voltage drives some relatively large sized ions (intercalants) into the van der Waals gap of 2DMs. Many individual nanosheets can then be isolated and dispersed in solvents and form a dispersion, which can be further printed into thin films for device applications, including photodetectors. The photodetectors based on solution-processed 2D semiconductors have shown ultra-high photoresponsivity. However, the properties of exfoliated semiconducting nanosheets are largely affected by their colloidal environments, such as solvents and surface ligands, leading to a broadly distributed and both deep and shallow lying trap states in the energy bands. Upon illumination, the photocarriers generated in the 2D light absorbers are captured by the traps and cannot be collected by the external circuit. The response time of the device is limited by the trap-filling process and the potential of 2DMs based photodetectors is not fully revealed yet.

To improve the photodetector performance, colloidal compatible dopants will be added to the dispersion to chemically treat the nanosheets. The dopants will bind to the nanosheet surface via local defects and reduce the trap states lying in the energy band. Functional thin films will be fabricated on pre-patterned gold coated substrates by solution-processing techniques, such as spin coating. The dispersion and thin film will be characterised to reveal the optical and electronic property variations before and after treatment. The performance of the photodetector will be evaluated regarding its photoconductivity, response time, photoresponsivity, and detectivity using a monochromatic light source.

The student will be able to acquire the state-of-the-art 2D material fabrication method, thin film formation techniques, and master optical and electrical characterisations.

**Capstone Project - September 2026**

**Jonathan Coleman**

**Title: Characterising the Electrical Properties of Ultrathin Nanosheet Networks Using Impedance Spectroscopy**

Printed networks of two-dimensional (2D) nanosheets have shown considerable promise for a range of electronic applications, including photodetectors, transistors, and light-emitting diodes. These networks consist of disordered arrays of nanosheets that are predominantly aligned within the plane of the film. Their electrical properties are typically limited by the resistance of the inter-nanosheet junctions. This junction resistance is, in turn, influenced by the morphological structure of the network and is strongly affected by disorder. Developing a clear understanding of the relationship between network structure, junction resistance, and overall electrical performance is therefore of significant importance.

In recent years, impedance spectroscopy has emerged as a powerful tool for characterising the electrical properties of nanosheet networks. In particular, this technique enables the measurement of junction resistance, the average resistance of individual nanosheets, and provides quantitative information about network disorder.

However, impedance spectroscopy is generally applied to relatively thick networks (i.e., thicknesses greater than tens of nanometres). This is because thinner networks tend to be more disordered, leading to an increase in resistance with decreasing thickness. These thickness-dependent effects complicate the analysis and interpretation of impedance spectroscopy data.

This project will investigate how the effective network thickness influences the measurement of junction and nanosheet resistance using impedance spectroscopy. The aim is to determine how impedance measurements scale quantitatively with nanosheet thickness, thereby enabling reliable extraction of junction resistance in ultrathin networks.

Solution-processed molybdenum disulfide ($MoS_2$) nanosheets will be used as a model system and deposited into networks via spin coating. The student will gain hands-on experience in nanosheet ink formulation, thin-film deposition, structural characterisation, and electrical measurements using impedance spectroscopy.

**AFM Thickness Measurement of Two-Dimensional Materials**

This project will study why atomic force microscopy (AFM) can give inaccurate thickness measurements for atomically thin materials such as graphene and $MoS_2$. In tapping-mode AFM, the measured step height depends not only on the true surface topography but also on tip–sample interactions such as adhesion, capillary forces, and trapped interfacial water. These effects can produce large variations in apparent thickness and even contrast inversion, where a monolayer appears lower than the substrate.[1-5]

The student will use an Asylum MFP-3D AFM to image 2D-material flakes under different operating conditions, varying parameters such as free amplitude and setpoint. The resulting topography and phase images will be analysed to determine how imaging conditions affect the apparent step height. A simple driven-oscillator model will then be used to interpret the results in terms of conservative and dissipative tip–sample interactions.

The aim is to identify the conditions that give the most reliable thickness measurements and to develop a clear physical explanation for AFM thickness anomalies in 2D materials. The project will give the student experience in nanoscale experimental techniques, data analysis, and the physics of oscillating systems and surface forces.


1. Haartsen, S., et al., *Humidity-controlled interactions and lifting of MoS2 on SiO2*. Journal of Physics-Materials, 2025. **8**(2).
2. Su, S.Q., J. Zhao, and T.H. Ly, *Scanning Probe Microscopies for Characterizations of 2D Materials*. Small Methods, 2024. **8**(11).
3. Bu, T., et al., *Thickness measurements of graphene oxide flakes using atomic force microscopy: results of an international interlaboratory comparison*. Nanotechnology, 2023. **34**(22): p. 225702.
4. Xiao, Y.P., et al., *Highly Accurate Thickness Determination of 2D Materials*. Crystal Research and Technology, 2021. **56**(6).
5. Godin, K., C. Cupo, and E.H. Yang, *Reduction in Step Height Variation and Correcting Contrast Inversion in Dynamic AFM of WS2 Monolayers*. Scientific Reports, 2017. **7**.

## Reliable Extraction of Contact Resistance in 2D $MoS_2$ Devices

This project will investigate how to measure and interpret contact resistance reliably in two-dimensional $MoS_2$ devices. Contact resistance is a major challenge in 2D electronics because the metal/semiconductor interface often dominates the total device resistance, masking the intrinsic transport properties of the $MoS_2$ channel. In practice, charge injection can be strongly influenced by Schottky barriers, Fermi-level pinning, and series resistance, so extracting meaningful contact parameters is not straightforward.[1-4]

The project will combine device fabrication, electrical characterisation, and temperature-dependent transport analysis. The student will fabricate simple back-gated $MoS_2$ field-effect devices, carry out current-voltage and gate-dependent measurements, and study how the electrical response changes with temperature. The data will then be analysed using contact-sensitive approaches such as transfer length method (TLM) and Schottky-based transport models. A key theme will be understanding when a device can be treated as a simple contact/channel system and when it behaves more like two back-to-back Schottky contacts with additional series resistance.

The aim is to establish a defensible workflow for distinguishing contact-limited from channel-limited transport, and for assessing the reliability and limitations of commonly used extraction methods in 2D semiconductors. The project offers hands-on training in nanodevice fabrication, semiconductor measurements, and experimental data analysis, and is well suited to students interested in condensed matter physics, nanotechnology, and electronic materials.


1. Wang, Z., et al., *Extraction and Analysis of the Characteristic Parameters in Back-to-Back Connected Asymmetric Schottky Diode*. physica status solidi (a), 2020. **217**(8): p. 1901018.
2. Wang, S., Z. Yu, and X. Wang, *Electrical contacts to two-dimensional transition-metal dichalcogenides*. Journal of Semiconductors, 2018. **39**(12).
3. Osvald, J., *Back-to-back connected asymmetric Schottky diodes with series resistance as a single diode*. physica status solidi (a), 2015. **212**(12): p. 2754-2758.
4. Kaushik, N., et al., *Schottky barrier heights for Au and Pd contacts to MoS2*. Applied Physics Letters, 2014. **105**(11).

**Machine Learning for Optical Identification of $MoS_2$ Thickness**

This project will explore the use of machine learning for rapid thickness identification of mechanically exfoliated $MoS_2$ flakes from optical microscope images. $MoS_2$ is a widely studied two-dimensional material whose optical and electronic properties depend strongly on layer number, so reliable thickness identification is an essential step in both fundamental research and device fabrication. While techniques such as AFM, Raman spectroscopy, and photoluminescence can provide accurate thickness information, they are relatively slow and less practical for large-area flake searching. Optical microscopy is much faster, but interpreting optical contrast by eye can be difficult, especially for few-layer regions and under varying imaging conditions.

In this project, the student will prepare $MoS_2$ samples by mechanical exfoliation onto $SiO_2$/Si substrates and acquire optical images under controlled microscope conditions. They will then write Python code to process the images, isolate flake regions from the substrate, and extract features such as colour and optical contrast.[1-5] These features will be used to train a simple machine-learning model to classify flakes by thickness, for example into monolayer, bilayer, trilayer, and thicker regions. The performance of the model will be evaluated against labelled data and, where available, reference thickness measurements.

The expected outcome is a practical analysis pipeline that demonstrates how machine learning can support faster and more objective identification of 2D material thickness from ordinary optical images. The project will give the student experience in sample preparation, optical microscopy, coding, data analysis, and applied machine learning, while also developing their understanding of the physics of optical contrast in thin layered materials.


1. Mahjoubi, S., et al., *Identification and classification of exfoliated graphene flakes from microscopy images using a hierarchical deep convolutional neural network*. Engineering Applications of Artificial Intelligence, 2023. **119**: p. 105743.
2. Joy, N.J., R.M. K, and J. Balakrishnan, *A simple and robust machine learning assisted process flow for the layer number identification of TMDs using optical contrast spectroscopy.* Journal of Physics: Condensed Matter, 2023. **35**(2): p. 025901.
3. Sanchez-Juarez, J., et al., *Automated system for the detection of 2D materials using digital image processing and deep learning.* Optical Materials Express, 2022. **12**(5): p. 1856-1868.
4. Dong, X., et al., *Deep-Learning-Based Microscopic Imagery Classification, Segmentation, and Detection for the Identification of 2D Semiconductors.* Advanced Theory and Simulations, 2022. **5**(9): p. 2200140.
5. Sterbentz, R.M., K.L. Haley, and J.O. Island, *Universal image segmentation for optical identification of 2D materials.* Scientific Reports, 2021. **11**(1): p. 5808.

# PROJECT 3 Does friction depend on how fast you slide? — Prandtl–Tomlinson thermal stick-slip

*9-week lab project · supervised by postdoc + grad student · CRANN Nanoscale Function Group*

*A 1928 mechanical model predicts that friction should have a specific logarithmic dependence on sliding velocity, driven by thermally activated stick-slip events. Testing this on a 2D-nanosheet coating connects classical tribology to statistical mechanics — and gives a direct preview of what will happen when the coating is placed in an aqueous environment.*

## THE PHYSICS QUESTION

The Prandtl–Tomlinson model describes a sliding tip as a damped spring that "sticks" in local atomic potential wells and thermally "slips" over energy barriers as it is dragged. Its signature experimental prediction is that the friction force depends logarithmically on sliding velocity: $F(v) = F_o + (kT/\lambda)\cdot\ln(v/v_o)$, where λ is a characteristic length scale (often interpreted as an atomic-scale jump distance), and kT is the thermal energy. This is one of the cleanest experimental fingerprints of thermally activated atomic-scale friction — and it predicts what the friction-versus-velocity curve should look like across many decades of v. Your project tests whether Tribocoined graphene on PET follows this law, extracts λ, and reasons about what that λ tells you about the atomic-scale friction mechanism.

## WHAT YOU WILL DO IN THE LAB

- Receive ~6 identically Tribocoined coupons.
- Fix the load at 10 mN.
- Vary sliding velocity from the minimum the tribometer can produce up to its maximum — ideally covering 2–3 decades in v.
- At each velocity, run multiple traces to beat down measurement noise; v-dependence is typically a weak effect (ln-scale), so data quality matters more than in the previous projects.
- Post-test AFM on wear tracks at the extreme velocities to confirm that the wear mechanism hasn't changed qualitatively across the sweep (otherwise you are not comparing like with like).

## WHAT YOU WILL ANALYSE

Plot F vs ln(v) and fit the Prandtl–Tomlinson form. From the slope (kT/λ), extract the characteristic length λ and compare it against physically reasonable candidates: the graphene lattice constant (a = 2.46 Å), the interlayer spacing of sheet-sheet contacts (c ≈ 3.4 Å), or a larger mesoscopic length set by flake-edge spacing in the Tribocoined network (tens of nm). The inferred λ tells you whether the friction bottleneck is atomic-scale sliding on pristine graphene basal planes (small λ) or flake-edge pinning events (large λ). If F is velocity-independent across your range, that's also a physical result — it means you're in the athermal regime, which places an upper bound on the relevant energy barriers.

## WHAT A SUCCESSFUL THESIS LOOKS LIKE

- **Guaranteed thesis outcome:** a friction-vs-velocity dataset at fixed load and wear-track imaging confirming consistent contact mechanics, with a direct comparison against the Prandtl–Tomlinson prediction.
- **Stretch outcome:** a clean logarithmic fit yielding a characteristic length λ, plus a defensible physical interpretation that distinguishes basal-plane sliding from edge-pinning. This would be a strong figure in a mechanism-of-friction paper and directly informs the aqueous-transition work SWIFT is proposing — hydration layers change λ in predictable ways, so your dry-air measurement becomes the reference baseline.

## STARTER READING (PICK 2–3 BEFORE YOU ARRIVE)


- Gnecco, E., Bennewitz, R., Gyalog, T., & Meyer, E., "Friction experiments on the nanometre scale," J. Phys. Condens. Matter 13, R619 (2001) — the canonical review of Prandtl–Tomlinson tests on real materials.
- Jansen, L., Hölscher, H., Fuchs, H., & Schirmeisen, A., "Temperature dependence of atomic-scale stick-slip friction," Phys. Rev. Lett. 104, 256101 (2010) — explicit test of the ln(v) prediction.
- Sang, Y., Dubé, M., & Grant, M., "Thermal effects on atomic friction," Phys. Rev. Lett. 87, 174301 (2001) — the theoretical argument for why ln(v), not v itself.
- Sinnott & Cross, Adv. Mater. (2024) — Tribocoining.


**SKILLS YOU WILL BUILD** — Thermally activated rate-process physics · multi-decade velocity measurements on the 2D nanoindenter · logarithmic fitting and error analysis · statistical-mechanics reasoning about sliding contacts · linking nanoscale physics to macroscopic friction measurements.

# PROJECT 2 How much material is removed per unit sliding? — Archard wear law with AFM

*9-week lab project · supervised by postdoc + grad student · CRANN Nanoscale Function Group*

*Classical wear theory (1953) says removed volume is proportional to load × sliding distance. You will test that directly on a 2D-nanosheet coating by running controlled sliding experiments and measuring the hole you leave behind.*

## THE PHYSICS QUESTION

Archard's Wear Law states $V = K \cdot (L \cdot d)/H$, where V is the volume of material removed, L is normal load, d is sliding distance, H is the hardness of the softer material, and K is a dimensionless wear coefficient specific to the sliding pair. For metallic and polymer systems K ranges from $10^{-8}$ to $10^{-2}$ depending on whether the contact is in mild or severe wear. No one has published an Archard coefficient for a Tribocoined 2D-nanosheet coating — partly because the wear mechanism may not even be Archardian (it might be flake-by-flake removal, edge-pinning failure, or tribochemical). Your job is to measure $V(L \cdot d)$, test whether Archard's linear scaling holds, and if it does, extract K for Tribocoined graphene on PET.

## WHAT YOU WILL DO IN THE LAB

- Receive ~6 identically Tribocoined coupons from the postdoc's prep run.
- Fix the load at 10 mN (middle of the 2D indenter's clean-friction range). Vary sliding distance from 1 mm up to ~100 mm in roughly 5 points on a log spacing.
- Also run a second sweep at fixed distance (say 50 mm) and vary load from 1 mN to 50 mN, to separately test V-vs-L and V-vs-d linearity.
- After each wear test, AFM-image the wear track and integrate the topography to extract wear volume. This is the measurement skill that makes this project intermediate rather than easy.

## WHAT YOU WILL ANALYSE

You'll have two linear-scaling predictions to test: V vs. d at fixed L, and V vs. L at fixed d. A proper Archard wear mechanism produces straight-line fits through the origin for both. Deviations from linearity tell a physical story — sublinear scaling at high load suggests a hardening response; superlinear suggests a catastrophic transition to severe wear; a nonzero intercept in V-vs-d suggests a "running-in" wear phase before steady-state sets in. You'll also compute K and compare against published values for graphite coatings ($K \approx 10^{-5}$ to $10^{-3}$), DLC ($K \approx 10^{-7}$), and PTFE ($K \approx 10^{-5}$).

## WHAT A SUCCESSFUL THESIS LOOKS LIKE

- **Guaranteed thesis outcome:** a quantitative wear-volume dataset with AFM-verified wear-track geometry for Tribocoined graphene on PET, plus a clear test of Archard's linear prediction in both L and d.
- **Stretch outcome:** a published-quality wear coefficient K for the coating, plus identification of the dominant wear mechanism (running-in, steady-state, or severe) from the shape of the V-vs-d curve. If the fit is clean, this becomes a citation-worthy number for any subsequent paper from the group.

## STARTER READING (PICK 2–3 BEFORE YOU ARRIVE)


- Archard, J.F., "Contact and Rubbing of Flat Surfaces," J. Appl. Phys. 24, 981 (1953) — the original paper, 6 pages, remarkably readable.
- Sinnott & Cross, Adv. Mater. (2024) —Tribocoining protocol.
- Holm, R., Electric Contacts (1946), §40 — the intellectual predecessor of Archard. Optional but satisfying.
- Williams, J.A., "Wear and wear particles — some fundamentals," Tribol. Int. 38, 863 (2005) — modern summary of what we do and don't know about wear mechanisms.


**SKILLS YOU WILL BUILD** — AFM topography and wear-volume integration · multi-parameter experimental design · quantitative comparison with published wear coefficients · reading a 1953 physics paper and applying its logic to a 2025 material · Python image analysis.

# PROJECT 1 Does friction scale linearly with load? — Amontons' Laws in a 2D coating

*9-week lab project · supervised by postdoc + grad student · CRANN Nanoscale Function Group*

*Test one of the oldest laws in physics (1699) against one of the newest materials (solid-state graphene coatings) — and find out whether a three-century-old textbook relation still holds when the contact is 10 atoms thick.*

## THE PHYSICS QUESTION

Amontons' First Law says friction force scales linearly with normal load (F = μN). Amontons' Second Law says friction is independent of the apparent contact area. Both were empirical 17th-century observations about wood and metals. For a novel "Tribocoined" 2D-nanosheet coating we have developed — where the contact is only 10's of atomic layers thick and where interlayer shear within the coating may matter as much as surface-surface sliding — it is not obvious either law should hold. Your project is to measure the F(N) relationship over nearly two decades of normal load and determine whether a single friction coefficient μ adequately describes Tribocoined graphene on PET, or whether you need a more sophisticated model (power-law, Hertz-contact, pressure-dependent).

## WHAT YOU WILL DO IN THE LAB

- Receive ~4–6 identically Tribocoined graphene-on-PET coupons (25 × 25 mm) produced by the postdoc in a single prep run, so coating variability is minimised.
- Run friction-force measurements on the 2D nanoindentation system across the load range 1 mN to 50 mN — roughly 8–10 points on a log spacing.
- At each load, collect 3–5 scratch traces to quantify measurement scatter.
- Post-test AFM imaging of one or two wear tracks to confirm that you have stayed in the mild-wear regime across the full load range (i.e., that the coating isn't catastrophically failing at high load).

## WHAT YOU WILL ANALYSE

You will plot friction force F versus normal load N on log-log axes, fit a power-law F = a·N^b, and compare the exponent b against 1 (Amontons). If b = 1, extract μ and compare against literature values for graphene (typical dry ambient: μ ≈ 0.1–0.3) and for PTFE (μ ≈ 0.04–0.1). If b ≠ 1, develop a physical argument for why — one candidate is a Hertz-like real-contact-area scaling that predicts b ≈ 2/3 for rigid spheres on soft substrates. A further optional layer is to test whether the data fits the Derjaguin offset form F = μN + $F_o$, where $F_o$ is an adhesion contribution.

## WHAT A SUCCESSFUL THESIS SHOULD LOOK LIKE

- **Guaranteed thesis outcome:** you will have an F(N) dataset spanning nearly two decades of load on a novel coating, with quantified experimental uncertainty and a clear statement of whether the data is consistent with Amontons' Law.
- **Stretch outcome:** a clean power-law fit at sufficient resolution to distinguish Amontons (b=1) from Hertz-contact-dominated (b=2/3) scaling, with a physical argument for which regime the coating sits in. This would become a figure in the group's aqueous-extension paper.

## STARTER READING (PICK 2–3 BEFORE YOU ARRIVE)


- Bhushan, Introduction to Tribology (2013), Chapter 5 — Friction basics. Just the first 20 pages; skim the rest.
- Sinnott, Y.C., & Cross, G.L.W., "Strain Recovery and Cohesive Lock-In of Nanosheet Thin Films Under High-Strain Compression," Advanced Materials (2024) — a Tribocoining paper.
- Mo, Y., Turner, K.T., & Szlufarska, I., "Friction laws at the nanoscale," Nature 457, 1116 (2009) — short, readable, and directly relevant.


**SKILLS YOU WILL BUILD** — Quantitative tribometry · log-log data analysis and power-law fitting in Python · AFM imaging of wear tracks · error propagation in multi-measurement datasets · reading a classical physics paper and turning it into an experimental hypothesis.

**Excitons in Molecular Crystals**

**Supervisor: Prof. Charles Patterson (Charles.Patterson@tcd.ie)**

Excitons are excited states of matter in which an excited electron remains bound to a hole. They are important in optoelectronics as they are often strong light absorbers and are the excitations by which light is absorbed in organic solar cells [1]. In this project you will learn to set up a model Hamiltonian to represent excitonic states in a molecular crystal. The Hamiltonian contains electron and hole hopping, electron-hole coulombic attraction and electron-phonon coupling.

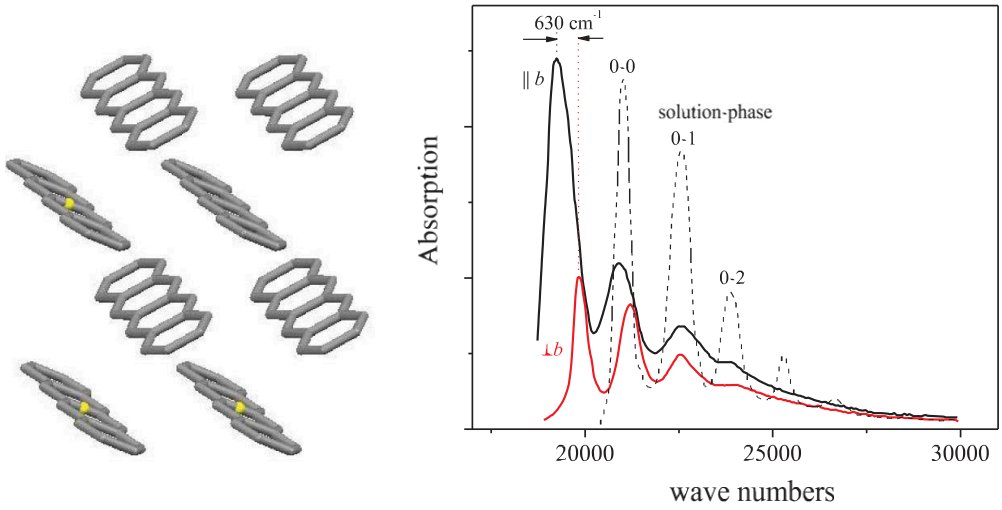



Figure: Structure of tetracene molecular crystal and its optical absorption spectrum [2]

In the project you will learn about second quantisation operators representing creation and annihilation of fermions (electron and holes) and bosons (phonons). You will write a Python script to set up the Hamiltonian and diagonalise it. You will learn to interpret eigenvectors of the model Hamiltonian and how to calculate the optical absorption spectrum from its eigenvectors and eigenvalues.

The project will be entirely theoretical and will use Python. It will suit someone who likes computing, coding and quantum mechanics. Some knowledge of chemistry at school or (preferably) junior undergraduate level would help, but is not essential for the project.

[1] *Expanded theory of H and H molecular aggregates: the effects of vibronic coupling and intermolecular charge transfer*, N. J. Hestand and F. C. Spano, Chem. Rev. **118**, 7069 (2018) doi.org/10.1021/acs.chemrev.7b00581

[2] *The nature of singlet excitons in oligoacene molecular crystals*, H. Yamagata et al. J. Chem. Phys. 134, 204703 (2011). doi.org/10.1063/1.3590871

**School of Physics Senior Sophister Research Project 2026-2027**

**"MAD" deposition of large molecular precursors for on-surface synthesis**

**Supervisor: Cormac McGuinness**
**E-mail: Cormac.McGuinness@tcd.ie**
**Materials – Materials**

A method named Matrix Assisted Deposition or "MAD" deposition has been introduced to allow for the ultraclean deposition of solvated large molecular weight precursor molecules onto atomically clean surfaces.[1] This bypasses restrictions on the molecular weight of heavier single molecules through organic molecular beam deposition where the necessarily higher thermal evaporation temperatures may damage, dissociate or fragment the molecules before they reach the intended surface. The student will implement or use a "MAD" deposition system to prepare heavy precursor materials for their on-surface synthesis into novel nanostructures.

On-surface synthesis methods allow for the creation of entirely novel periodic nanostructures on surfaces derived from molecules rationally designed to form networks which form through temperature assisted chemical processes. One dimensional nanoribbon systems, such as graphene nanoribbons (GNR), or 2D networks can be constructed from differing precursor molecules. Growth surfaces are typically single crystal noble metal surfaces such as Au(111), but small and lower molecular weight molecules work best when thermally evaporating from Knudsen cells in an organic molecular beam deposition methods which all occur in ultraclean ultra-high vacuum (UHV) environments. work Here precursors derived from the well-known transition metal porphyrins will introduce interesting properties of the nanostructures.

The project will involve training in ultra-high vacuum (UHV) systems and getting experience of surface science techniques, the use of x-ray photoemission spectroscopy (XPS) instruments and the participation in scanning tunnelling microscopy (STM) measurements. The materials in question will be large molecular weight porphyrin-based precursors provided by the Senge group. Good technical abilities, steady hands, excellent hand-eye coordination and a careful informed approach are essential for a student engaged in this work.

[1] McCurdy R D et al "*Synergetic Bottom-Up Synthesis of Graphene Nanoribbons by Matrix-Assisted Direct Transfer*" J. Am. Chem. Soc., **143** 4174–8, 2021

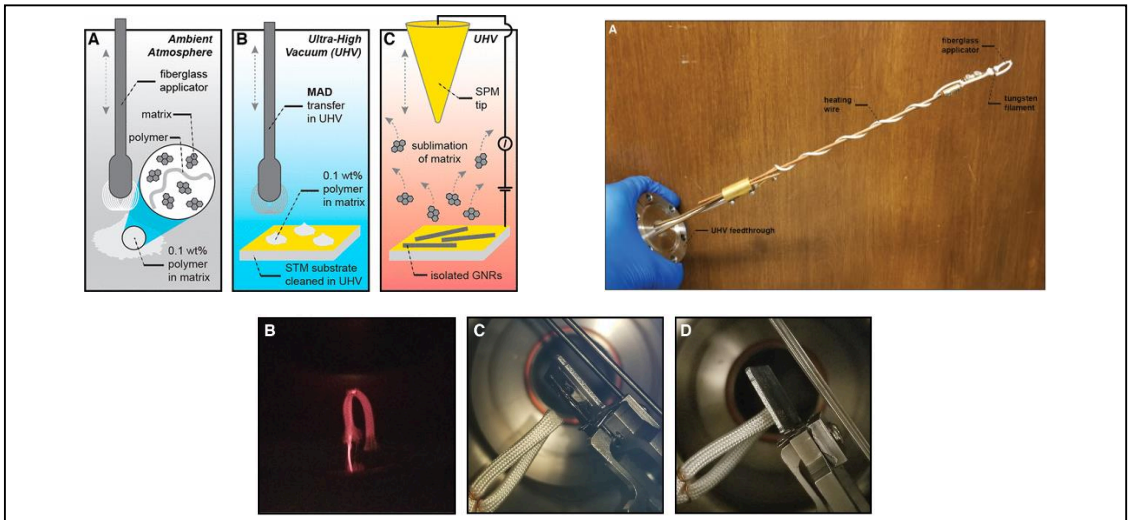



Figure 1:Upper left: The "MAD" process as per McCurdy et al; (A) the proposed MAD applicator; Lower: Thermally cleaning the applicator (B), before applying the dosed applicator to a sample (C,D).

**School of Physics Senior Sophister Research Project 2026-2027**

**Reduction/oxidation study of metal oxide thin films on ruthenium surfaces – investigation into lowered metal oxide reduction due to bimetallic catalysis**

**Supervisor: Cormac McGuinness**
**E-mail: Cormac.McGuinness@tcd.ie**
**Materials / Energy – Experimental project.**

Solid oxide fuel cells (SOFC) in principle require only air as a source of oxygen, which undergoes an oxygen reduction reaction (ORR) catalysed by the cathode electrode. This ORR can be expressed in simple terms as a dissociation/reduction interaction between gaseous oxygen and the cathode surface, converting $O_2$ into negatively charged oxygen ions. High operational temperature (>800 °C) required for SOFC cathodes have been a barrier to widespread SOFC use. A research goal would be to improve SOFC efficiency via alternative cathode materials capable of catalysing ORR at lower temperatures.

Intriguing results achieved with manganese/ruthenium cathode surfaces show evidence for unusual metal oxide ORR at temperatures as low as 500 °C, with earlier literature results indicating that ruthenium may influence nickel oxides similarly. This project seeks to further the understanding of this behaviour for either manganese or nickel and further our understanding of this bimetallic catalysis and destabilisation of the Ni-O or Mn-O bonding.

The investigation in this project would deposit monolayers (ML) or several monolayers of nickel or manganese onto a single crystal Ru(0001) surface or sputter-deposited Ru thin film. These layers would be oxidised to NiO or MnO and the subsequent in vacuum reduction to Ni or Mn and the temperature dependence of this reduction would be studied. This investigation will occur via ultra-high vacuum (UHV) surface science analysis techniques, firstly by Auger Electron Spectroscopy (AES) and low energy electron diffraction (LEED), followed by x-ray and ultraviolet photoemission spectroscopies (XPS and UPS) when part of a fully in-situ growth and analysis experimental procedure.

The basic three stages of the ideal experiment would involve the cleaning and preparation of a clean Ru(0001) surface, the in-situ growth of Ni or Mn layers on that surface, controlled $O_2$ exposure to oxidise, followed by high temperature UHV annealing cycles to ascertain the lowest temperature at which the oxygen reduction reaction can be achieved. Crucially, all stages of sample cleaning, sample growth, $O_2$ catalysis and sample analysis would be performed in-situ within UHV.

If successful, XPS and UPS at each step could evaluate the validity of the *d*-band model of catalysis to this Ni/Ru or Mn/Ru system and to evaluate the result for differing thin films (<6ML) and thicker islanded growths. [e.g. Mn layers grow pseudomorphically with the underlying Ru surface until islanding occurs after 6 ML.] Results from the single crystal Ru(0001) surfaces will be compared to past results and studies being undertaken this summer obtained from Mn on Ru thin films generated by atomic-layer-deposition or by binary alloys respectively.

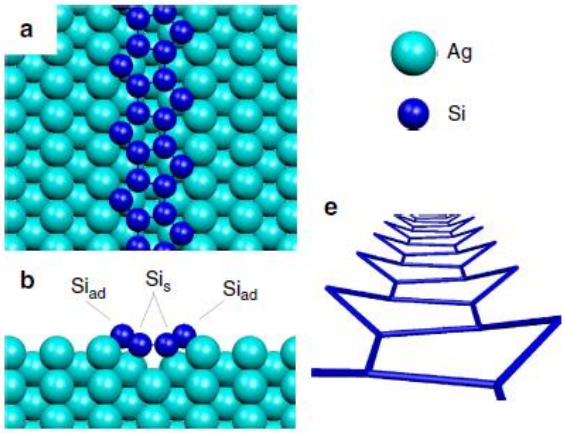
The student will become skilled in many aspects of surface science, vacuum technology and analytical techniques inclusive of x-ray photoemission spectroscopy. The project goals may need to altered depending upon equipment availability. If the necessary equipment is not available during the project period then this may become more of a data analysis or simulation project.

**NOTE: this experimental project is subject to the availability of the necessary equipment in September 2026.**

**School of Physics Senior Sophister Research Project 2026-2027**

**The measurement of the reflectance anisotropy spectrum (RAS) arising from penta-silicene nanoribbons formed on Ag(110)**

**Supervisor: Cormac McGuinness**
**E-mail: Cormac.McGuinness@tcd.ie**
**Materials / Energy – Experimental project.**




This project is to measure for the first time the optical anisotropy due to penta-silicene nanoribbons that can be formed on Ag(110) surfaces. It has recently been shown by Cerda et al. that a monolayer of silicon evaporated onto Ag(110) surfaces can form a variety of penta-silicene nanoribbons [1]. These nanoribbons form parallel to the Ag [110] rows displacing one of the surface rows i.e. of the missing row reconstruction, where the silicon forms a chain of distorted pentagons within the missing row troughs (**a**,**b**). Each pentagon consists of four co-planar silicon atoms in the trough with the fifth silicon adatom buckling the planarity of the pentagon (**e**). These one-dimensional silicon surface nanostructures have been controversial. Evidence from Cerda et al [1] for both single and double silicene penta-nanoribbon formation now gives confidence that the above is an accurate picture.
This experimentally challenging project involves the preparation of ultra-clean Ag(110) surfaces in ultra-high vacuum, verification of this via low energy electron diffraction (LEED) and by Auger electron spectroscopy (AES), the calibration and evaporation of <1ML of Si onto these surfaces (to be verified via AES). The goal being the measurement of the anisotropic optical properties of the penta-silicene nanoribbons *as measured in situ during the penta-silicene nanoribbon formation* via reflection anisotropy spectroscopy (RAS) and subsequent structural measurement by LEED. Earlier surface differential reflectance spectroscopy (SDRS) measurements by Borensztein et al [2] were obtained for what should be the same system described by Cerda et al. but as of yet no direct RAS measurement has been acquired from this penta-silicene system. The objective is to complete such measurements. The student will become skilled in many aspects of surface science, vacuum technology, surface optical linear spectroscopy and analytical techniques.

**NOTE: this experimental project is subject to the availability of the necessary equipment in September 2026.**

[1] J. I. Cerda et al, Nature Communications, **7**, 13076, 2016 10.1038/ncomms13076
[2] Y. Borensztein et al., Phys. Rev. B, **89**, 245410 (2014) 10.1103/PhysRevB.89.245410

**School of Physics Senior Sophister Research Project 2026–2027**

**Development of an Angle-Resolved X-ray Photoelectron Spectroscopy (AR-XPS) Depth Profiling Application**

**Supervisor:** Richard Gubo / Cormac McGuinness

**E-mail: gubor@tcd.ie**

**Materials** / Surface Science – Experimental & Computational Project

Angle-resolved X-ray photoelectron spectroscopy (AR-XPS) is a powerful non-destructive surface analysis technique capable of probing the chemical composition of materials as a function of depth within the first few nanometers of a surface. Unlike conventional sputter depth profiling, AR-XPS preserves delicate interfaces and allows chemically sensitive analysis of thin films, oxides, semiconductors, catalysts, and layered nanostructures.

The aim of this project is to develop an interactive data application in streamlit for quantitative AR-XPS depth profile reconstruction using Tikhonov or MEM (Maximum Entropy) regularization methods. The application will allow users to import multi-angle XPS datasets, reconstruct concentration depth profiles, optimize reconstruction parameters, and visualize layered structures in an intuitive graphical interface. The application will be validated on available literature data.

The project will combine surface science, numerical modelling, and scientific programming. The reconstruction algorithm will model the attenuation of photoelectrons emitted from different depths and solve the inverse problem associated with AR-XPS analysis using regularized optimization approaches. The student will investigate factors influencing reconstruction quality including attenuation lengths, elastic scattering effects, regularization parameters, and the influence of initial guess models[1].

Potential software features include:

• Reconstruction of concentration depth profiles from multi-angle datasets.

• Adjustable attenuation length models using IMFP or EAL approaches.

• Automatic optimization of regularization parameters.

• Visualization and export of high-quality depth profile plots.

Experimental datasets may include metal oxides, catalytic surfaces, semiconductors, or layered materials measured under ultra-high vacuum (UHV) conditions. If successful, the final application could become a reusable AR-XPS analysis tool and contribute toward future research publications or open-source scientific software development.

The student will gain experience in XPS/AR-XPS analysis, numerical optimization, Python scientific programming, and surface/interface physics.

---

[1] Paynter, R. (2008). An ARXPS primer. *Journal of Electron Spectroscopy and Related Phenomena*, *169*(1), 1–9. https://doi.org/10.1016/j.elspec.2008.09.005

Murdoch, B. J., & McCulloch, D. G. (2023). Surface analysis insight note: Straightforward concentration depth profiling by angle-resolved X-ray photoelectron spectroscopy using a Tikhonov regularization algorithm. *Surface and Interface Analysis*, *55*(9), 658–664. https://doi.org/10.1002/sia.7240

# Optical Characterisation of Transparent Conducting Oxides using Spectroscopic Ellipsometry

The Applied Physics Research Group chaired by Prof. Igor Shvets is renowned as one of the leading international groups in the synthesis and application of metal oxide thin films. It conducts interdisciplinary research across a wide range of applied physics projects, encompassing materials science, photonics, and nanoscale phenomena. Through a combination of development, experiment, modelling, and advanced characterisation, the group's quest is to understand and control physical properties at the microscopic level for technological innovation.

This project introduces the student to Spectroscopic Ellipsometry and the analysis of bulk and thin film (nanometer scale) materials with a particular focus on Transparent Conducting Oxides, such as Cu2O and ZnO for example. In addition, the project will involve both thin film growth and X-ray Diffraction (XRD) characterisation. The project centres on a genuine materials physics problem; how and why optical properties will evolve from bulk materials to thin and ultrathin film systems.

The project offers significant scope for independent investigation and critical comparison with published literature and has the potential to contribute to ongoing research within the Applied Physics Group. Furthermore, ellipsometry, XRD and thin film growth are critical in the semiconductor industry.

Working in the Optical Analysis Laboratory the student will develop proficiency with the Woollam M2000, a state-of-the-art Ellipsometer. The project will progress to full optical characterisation of advanced materials through measurement and optical modelling, including the extraction of the complex refractive index and dielectric function as a function of wavelength.

The student will investigate features in the data arising from underlying physical mechanisms, such as interband transitions, free-carrier (Drude-like) behaviour, excitonic peaks, and anisotropy where present.

# Characterising copper(II) oxide based memristors for neuromorphic computing applications.

**School of Physics and AMBER/CRANN,**
**Supervisor; Prof Igor V. Shvets ivchvets@tcd.ie**
**Co-supervisor; Dr. Varun Ranade vranade@tcd.ie**

Memristors are two-terminal electronic devices whose resistance can be tuned and retained, allowing information to be stored directly within their resistance state [1-2]. This unique property makes them powerful building blocks for brain-inspired neuromorphic computing, in which memory storage and computation take place at the same physical location. By contrast, conventional von Neumann architectures separate memory (RAM/cache) from the processing unit (CPU), forcing a constant shuttling of data between the two. This back-and-forth is widely recognised as a fundamental bottleneck of modern computing, incurring significant time and energy costs. Memristor-based chips, inspired by the way biological neurons co-locate computation and memory, sidestep this bottleneck and promise computing platforms that are simultaneously faster and far more energy-efficient than their conventional counterparts [3-4].

At its core, a memristor is a metal-dielectric-metal stack in which an applied electrical stimulus drives resistive switching within the dielectric, with the resulting resistance state encoding the stored information. This project focuses on copper(II) oxide memristors with gold electrodes. The aim is to emulate the behaviour of a biological neuronal synapse through a systematic suite of electrical characterisation protocols and to rigorously quantify the resulting performance metrics. Copper(II) oxide is a well-studied p-type transparent conducting oxide that can be readily deposited by RF sputtering at low cost, making it a particularly attractive candidate for the next generation of energy- and cost-efficient memristive devices.

1. D. B. Strukov, G. S. Snider, D. R. Stewart, and R. S. Williams, *The missing memristor found.* Nature, 2008. 453(7191): p. 80-83.
2. L. Chua, *Memristor-The missing circuit element.* IEEE Transactions on Circuit Theory, 1971. 18(5): p. 507-519.
3. Kim, W., Menzel, S., Wouters, D. J., Guo, Y., Robertson, J., Roesgen, B., ... & Rana, V. (2016). Impact of oxygen exchange reaction at the ohmic interface in Ta 2 O 5-based ReRAM devices. *Nanoscale*, *8*(41), 17774-17781.
4. Funck, Carsten, and Stephan Menzel. "Comprehensive model of electron conduction in oxide-based memristive devices." *ACS Applied electronic materials* 3.9 (2021): 3674-3692.

## Metal-Insulator Transition in Vanadium Oxide.

**Supervisor: Prof. Igor Shvets**

**Co-supervisor: Dr. Amy McGlinchey**

$VO_2$ is a strongly correlated transition metal oxide that exhibits a reversible metal–insulator transition (MIT) near 68 °C, accompanied by significant changes in its electrical, optical, and structural properties. Due to these characteristics, $VO_2$ thin films are of considerable interest for applications in smart windows, electronic switching devices, and neuromorphic technologies. In this project, $VO_2$ thin films prepared using two different deposition techniques, molecular beam epitaxy (MBE) and magnetron sputtering, will be systematically compared.

The study will focus on the structural and physical characterisation of the films in order to investigate how the deposition method influences material quality and phase-transition behaviour. X-ray diffraction and X-ray reflectivity measurements will be used to determine crystal structure, phase purity, film thickness, and interface quality, while Raman spectroscopy will provide information on the phase composition. The MIT will be examined through temperature-dependent measurements to compare transition temperature and switching behaviour between the two film types.

By correlating the structural and spectroscopic properties with the observed MIT characteristics, this work aims to evaluate the strengths and limitations of MBE and magnetron sputtering for the growth of high-quality $VO_2$ thin films.

# Development of $SiO_2$ Thin-Film Deposition by Electron-Beam PVD for Memristor Applications

**School of Physics and AMBER/CRANN,**

**Supervisor:** Prof Igor V. Shvets ivchvets@tcd.ie

**Co-supervisor:** Dr. Igor Chunin chunini@tcd.ie

One of the primary focuses of Igor Shvets lab is development of novel memristors devices with tunable volatility which represent a promising platform for neuromorphic computing and adaptive electronics[1]. We systematically investigate Ag/$SiO_2$/Au structures to elucidate the physics of silver filament evolution, revealing the asymmetric interplay between drift-dominated formation and diffusion-dominated rupture processes[2].

Over the past year several key developments have significantly enhanced the research environment. Professor Igor Shvets has recently acquired a state-of-the-art ultra-high vacuum (UHV) molecular beam epitaxy (MBE) system, equipped with two high-power electron-beam evaporators (twelve pockets in total). This system enables the precise physical vapour deposition (PVD) of complex alloys with controlled stoichiometry and defect density capabilities central to engineering the targeted memristive oxide structures.

During e-beam evaporation, $SiO_2$ dissociates into sub-oxides $SiO_{2-x}$ and oxygen gas, resulting in formation of oxygen-depleted non-stoichiometric films. This appeared to be the case for the new MBE system as well, which yields $SiO_{2-x}$ films when deposited from the crucible with $SiO_2$ pallets. To overcome this challenge and achieve stoichiometric, highly transparent $SiO_2$ it is standard practice to inject a small amount of oxygen (typically 1 x $10^{-4}$ Torr or 5-10% $O_2$) during the deposition[3]. The system is due to be upgraded to specifically introduce oxygen gas-dosing and substrate-heating capabilities that would allow for growth of oxide films suitable for memristor fabrication. In this project the experiments on $SiO_2$ e-beam depositions in high-vacuum environment with various $O_2$ content and substrate temperature will be conducted in order to establish the best parameters of the films growth via post-growth ex-situ XRR/XRF/XRD[3]/XPS[4] analysis and electrical measurements.

*References:*

[1] **Wang, R**.; Yang, J.-Q.; Mao, J.-Y.; Wang, Z.-P.; Wu, S.; Zhou, M.; Chen, T.; Zhou, Y.; Han, S.-T. Recent Advances of Volatile Memristors: Devices, Mechanisms, and Applications. *Advanced Intelligent Systems* **2020**, *2*, 2000055.

[2] **Varun Ranade**, William Veldhoen, Felix Gibbins, Sajal Shradha, Chris Murray, Igor Chunin, David McClosekey, Igor Shvets. Threshold Dynamics of Silver Filament Formation and Rupture in Ag/$SiO_2$/Au Memristors. P*reprint Zenodo* **2026**, DOI: 10.5281/zenodo.19291920

[3] Huang, Boris & Liu, Yuan-Shing & Chen, Yen-Ming & Huang, Ming-Chin & Moo-Chin, Wang. Effect of oxygen pressure on the microstructure and properties of the $A_{l2}O_3$–$SiO_2$ thin films deposited by E-beam evaporation. *Surface and Coatings Technology* **2006**, 200. 3309-3313. DOI: 10.1016/j.surfcoat.2005.07.032.

[4] R. Alfonsetti, L. Lozzi, M. Passacantando, P. Picozzi, S. Santucci, XPS studies on SiOx thin films, Applied Surface Science, Volumes 70–71, Part 1, 1993, Pages 222-225, ISSN 0169-4332, DOI:10.1016/0169-4332(93)90431-A.

# Multilayer p-type transparent conducting oxides: Pristine and nitrogen doped $Cu_2O$

**School of Physics and AMBER/CRANN,**
**Supervisor; Prof Igor V. Shvets ivchvets@tcd.ie**
**Co-supervisor; Dr. Brian Walls wallsbc@tcd.ie**

Transparent Conducting Oxides (TCOs) are essential for optoelectronic devices such as flat-panel displays, touchscreens, and solar cells by acting as transparent electrodes. The optimization of n-type semiconductor TCOs is a well-explored field, with materials such as Sn:$In_2O_3$ (ITO) and InGaZnO (IGZO) displaying impressive conductivities and visible transparency [1]. As a result, these materials are widely used in thin film transistors, photovoltaics and gas sensors. In comparison, the performance of p-type TCOs lags behind. Synthesizing p-type TCOs with sufficiently high performance would result in a number of important applications, such as the transparent p-n junction and an increase in the efficiency of OLEDs. The poor performance of p-type TCOs is typically due to unsatisfactory charge carrier concentrations or hole mobilities intrinsic to the O 2p nature of the valence band maxima in many oxide materials [2]. An interesting approach towards improving p-type TCO performance is layering two p-type materials, each with different desirable characteristics, for example high mobility and high carrier concentration. In theory, if the layers are sufficiently thin (<10nm), the structure as a whole can exhibit the desired properties of the constituent layers.

$Cu_2O$ was one of the first p-type semiconductors to be discovered [3] and can exhibit a huge mobility of 200$cm^2$/Vs proportional to the crystalline quality [4]. However, the carrier concentration is typically $10^{14}$-$10^{15}$ $cm^{-3}$ and is inversely proportional to the hole mobility resulting in $Cu_2O$ bordering on being an insulator. Doping $Cu_2O$ with nitrogen drastically increases the carrier concentration while reducing the mobility [3]. In Prof. Shvets group led by Dr. Walls, highly crystalline $Cu_2O$ is grown by magnetron sputtering on lattice matched MgO substrates. The $Cu_2O$ films are epitaxial; the growth orientation is controlled by the substrate orientation; and films as thin as 5nm have been synthesized. In this project, nitrogen doping of these films will be performed. The incorporation and concentration of nitrogen will be examined by X-ray photoelectron spectroscopy, X-ray diffraction and X-ray fluorescence. Furthermore, the changes in electrical and optical properties will be explored as a function of nitrogen doping. A secondary objective is to grow multilayers consisting of pristine and nitrogen doped Cu2O layers, corresponding to high mobility and high carrier concentration layers. The electrical and optical properties of the multilayer will be compared to the constituent layers.

1. Fleischer, Karsten, et al. "Quantifying the performance of P-type transparent conducting oxides by experimental methods." Materials 10.9 (2017): 1019.
2. Zhang, Kelvin HL, et al. "P-type transparent conducting oxides." Journal of Physics: Condensed Matter 28.38 (2016): 383002.
3. Grondahl, Lars Olai. "The copper-cuprous-oxide rectifier and photoelectric cell." Reviews of Modern Physics 5.2 (1933): 141.
4. Singh, Vivek, et al. "CVD-deposited $Cu_2O$ thin films with a record Hall hole mobility of 263 $cm^2$ $V^{-1}s^{-1}$ and field-effect mobility of 0.99 $cm^2$ $V^{-1}s^{-1}$." Journal of Materials Chemistry C 11.22 (2023): 7356-7366.
5. Rezek, Jiří, et al. "Ultra-low-resistivity nitrogen-doped p-type Cu2O thin films fabricated by reactive HiPIMS." Applied Surface Science (2025): 164380.

**Quantifying the relationship between the morphology and mobility of printed nanosheet networks: Towards high performance printed devices.**

**Supervisor:** Jonathan Coleman

Printed networks of two-dimensional (2D) nanosheets are important components in a wide range of electronic technologies, including transistors, photodetectors, and light-emitting devices. Maximising the charge-carrier mobility of these networks is crucial for improving device performance. Recently, we have identified clear correlations between device mobility and various parameters that describe the uniformity of nanosheet networks. Understanding these correlations could provide a route to optimising printing processes, enabling the production of highly uniform films with exceptionally high mobility.

A recently developed technique in our group allows network uniformity to be measured quickly and simply using an optical transmission scanner. This method provides optical measurements of film thickness at thousands of locations across a sample, enabling detailed statistical analysis of network morphology and uniformity.

This project will use this technique to quantitatively investigate how different deposition and printing methods influence the uniformity of networks of $MoS_2$ nanosheets. In addition, it will explore the relationship between network morphology and electrical properties such as conductivity and mobility.

Networks will be fabricated using a range of deposition techniques, including Langmuir–Schaefer deposition, spin coating, and spray coating. For each method, key processing parameters will be systematically varied, while the scanner will be used to measure the resulting thickness distributions. This will allow us to determine how quantities such as the mean film thickness and, more importantly, the thickness variance depend on deposition conditions.

For example, by characterising sequentially deposited layers and analysing how thickness variance evolves with layer number, we will be able to quantify correlations between individual layer thicknesses (i.e. covariance). Such measurements will provide insight into the statistical processes governing film growth. In spin-coated networks, we will investigate how the mean thickness and thickness variance depend on parameters such as ink concentration and spin speed. This will allow us to identify conditions that minimise film non-uniformity, while also revealing fundamental relationships between the mean thickness and its variance, including whether certain scaling relationships are conserved under specific deposition conditions.

The project will generate a comprehensive set of quantitative relationships linking deposition conditions to network uniformity. For a subset of the films produced, detailed electrical characterisation will also be carried out. This will enable us to establish direct relationships between electrical performance metrics, such as conductivity and mobility, and morphological parameters, such as thickness variance and the ratio of thickness variance to mean thickness.

Taken together, these results will provide a roadmap for the optimisation of nanosheet network fabrication and printed electronics more broadly. By identifying the morphological characteristics that enable high electrical performance, the project will contribute to the development of next-generation printed electronic devices with significantly improved functionality and efficiency.

# Surface-Dependent Superconductivity in $UTe_2$: An Atomic-Scale Study

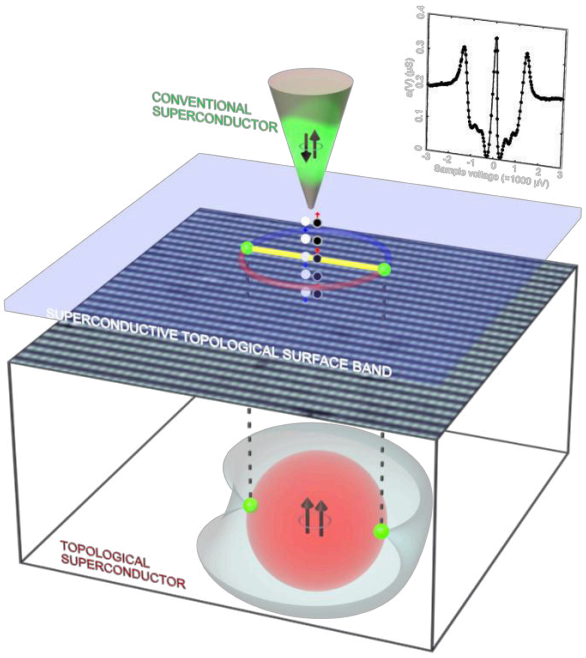
**Supervisor: Asst. Prof. Kuanysh Zhussupbekov**
**Email: kzhussup@tcd.ie**

Uranium ditelluride ($UTe_2$) was first identified as a superconductor in 2019 [1] and has since emerged as a leading candidate for spin-triplet, odd-parity topological superconductivity. Despite extensive research, its superconducting order parameter remains unresolved. Recent scanning tunnelling microscopy (STM) studies have revealed that $UTe_2$ hosts a superconductive topological surface band (TSB) [2] and distinct quasiparticle interference (QPI) patterns [3], enabling insights into its pairing symmetry. These results suggest a time-reversal-symmetric, odd-parity superconducting state with a nodal structure aligned along the crystal axes.

However, all experimental studies to date have focused exclusively on the naturally cleaving (0–11) surface. It remains unknown whether other crystallographic surfaces exist and, if so, whether they exhibit different superconducting or topological properties. This project will explore previously unstudied surfaces of $UTe_2$, investigating how the superconducting electronic structure depends on surface orientation. Since the projection of the bulk order parameter onto a given surface determines the observable surface states, different crystal planes may host distinct quasiparticle spectra and topological features.

## Objectives

- Identify and characterise alternative crystallographic surfaces of $UTe_2$
- Investigate whether superconductivity depends on surface orientation
- Map quasiparticle interference (QPI) patterns on different surfaces
- Examine how surface orientation affects nodal structure and electronic states
- Explore the possibility of new or hidden superconducting phases




## References

[1] S. Ran, C. Eckberg, Q.-P. Ding, Y. Furukawa, T. Metz, S. R. Saha, I.-L. Liu, M. Zic, H. Kim, J. Paglione, and N. P. Butch, "Nearly ferromagnetic spin-triplet superconductivity in $UTe_2$," *Science* **365** (2019), 684–687.

[2] Q. Gu, S. Wang, J. P. Carroll, K. Zhussupbekov, C. Broyles, S. Ran, N. P. Butch, J. A. Horn, S. Saha, J. Paglione, X. Liu, J. C. Séamus Davis, and D.-H. Lee, "Pair wave function symmetry in $UTe_2$ from zero-energy surface state visualization," *Science* **370** (2025), 938–942.

[3] S. Wang, K. Zhussupbekov, J. P. Carroll, B. Hu, X. Liu, E. Pangburn, A. Crepieux, C. Pepin, C. Broyles, S. Ran, N. P. Butch, S. Saha, J. Paglione, C. Bena, J. C. Séamus Davis, and Q. Gu, "Odd-parity quasiparticle interference in the superconductive surface state of $UTe_2$," *Nature Physics* **21** (2025), 1555–1562.

## Vacuum Chamber Molecular Water Contaminant Control

Prof. Lewys Jones & Dr Jon Peters, Ultramicroscopy Research Group

(www.tcd.ie/Physics/research/groups/ultramicroscopy/)

**Keywords:**

Vacuum chambers, residual moisture, water contamination, dehimidification.

**Abstract:**

Many experimental physics techniques require instruments that include a vacuum chamber. These are typically large aluminium or stell chambers with with many sealed ports used for sample-exchange, power, gas, mechanical interaction, fibre-optic feedthrough or electrical stimulation (Figure 1). These ports are typically sealed with rubber o-rings or copper metal gaskets, but no vacuum seal can ever be perfect and the small (but non-zero) leak-rate has two effects; firsly, that pumping must be continually applied to maintain a good vacuum, and second, that contaminants including water vapour can leak into the chamber. When the makeup of the residual gasses in a vacuum chamber are analysed, a profile of the contaminants is obtained (Figure 1).

*Figure 1. Example of a typical steel vacuum chamber with multiple access ports.*

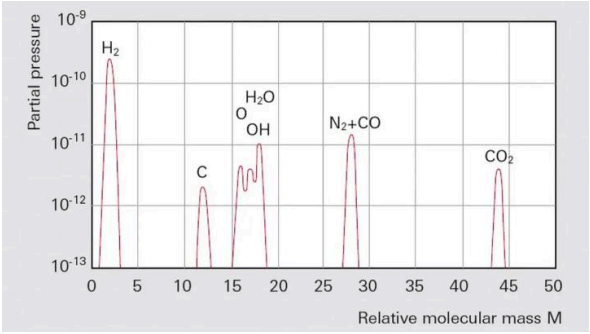



*Figure 2. Typical residual gas profile for a mixture of atmospheric air, water, and hydrocarbon contaminants.*

This water moisture can cause several problems, including: damage to the equipment, excess load/wear on vacuum pumps, chemical reactions with specimens under study, unwanted ice buildup on cryogenic fittings, or generate false readings. This project will evaluate the potential for new solid-state dehumidification technology with no moving parts, in a secondary atmospheric shield region around the vacuum chamber.

**Expected Outcomes:**

During this project, with the support of others in the research group, the student will:

- Design and assemble a secondary enclosure around a small test vacuum chamber.
- Install the solid-state dehumidifier including calculating the energy requirements of the system.
- Take baseline vacuum hygiene measurements and repeat these after moisture removal.
- Compare the findings and extrapolate to a full-size system's performance.

If the research progresses expected, we aim to write a research paper on this new technology.

**Further Details:**

The project and desk will be based in the Advanced Microscopy Laboratory (www.tcd.ie/crann/aml). The ideal student will have an interest in practical work, 3D printing or mechanical design.

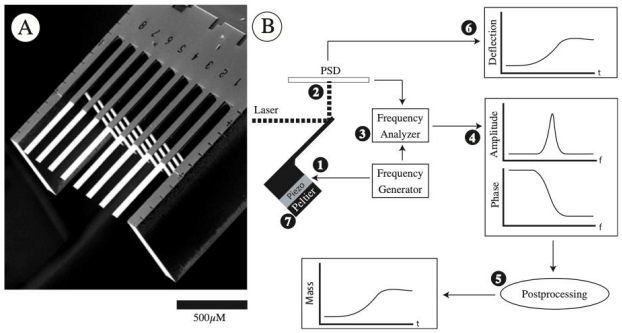
**School of Physics Senior Sophister Research Project 2026**

# Biomolecular interaction analysis graphical user interface (GUI)

**Prof. Martin Hegner**
**hegnerm@tcd.ie**

The Hegner Group pioneered the development of label-free biomolecular diagnostic nanomechanical platforms and introduced diagnostic assays in the field of genomics, protoeomics and vaccine analytics [1-3]. The dynamic mode detection of picograms of target molecules allows a rapid and personalized. In the dynamic mode the mass increase on the cantilever due to ligand adsorption is measured by tracking the eigenfrequency at higher harmonics. (ii) In the static mode, conformational changes of receptors, charge effects and/or sterical competition between different ligand molecules on the sensor surface lead to a bending of the cantilever. A in house developed National Instruments LabVIEW software package enables the precise control of the measurement devices through analog/digital, frequency generations and digitising hardware. We utilize a LabVIEW software script for the comprehensive analysis of such data.
This unique combination of different physically measured properties in parallel needs an update of software for efficient data analysis. Furthermore, some techniques do not record directly the desired parameters versus time and have to be first post-processed after the experiment before a conclusive discussion can be performed. The availability of three different cantilever array designs requires a modular software database that can be integrated for future designs. Dynamic mode data the frequency/phase is occurring in liquids with variable density/viscosity and is tracked directly by a phase lock loop system (PLL) or by recording response spectra (amplitude, phase) in dependence of the excitation frequency. From the raw data, various properties can be extracted such as damping and the absolute mass of the ligand bound to the cantilever.

In this senior sophister project, the student will acquire nanomechanical experimental data sets that subsequently will be analyzed with the upgraded software package for cantilever array sensing measurements. The LabVIEW data analyzer software needs to be further programmed to automatize the data handling with the different nanomechanical geometries, variation of hydrodynamics and changing environmental variables. Solid programming skills in Python required to facilitate transition towards this graphical programming interface within the SS project.




a) Illustration of nanomechanical sensor array and b) work flow of the data acquisition that provides deep insights into mechanical changes occurring during diagnostic measurements.

(1) T. Braun, F. Huber, M K. Ghatkesar, N. Backmann, H. P. Lang, Ch. Gerber, and M. Hegner (2007) **Sens. Act. B -Chemical,** 128, 75-82
(2) M. Walther, P.M. Fleming, F. Padovani, M. Hegner, (2015) An optimized measurement chamber for cantilever array measurements in liquid incorporating an automated sample handling system **EPJ Techniques and Instrumentation** 2:7, DOI 10.1140/epjti/s40485-015-0017-7
(3) Brunetti, G., De Pastina, A. and Hegner, M. (2021) Nanoscale Advances 3, 6903–6911

**School of Physics Senior Sophister Research Project 2026**

# Can interfacial stress changes of sensors affect the mass detection biomolecular interactions?

**Prof. Martin Hegner**
**hegnerm@tcd.ie**

The Hegner Group pioneered the development of label-free biomolecular diagnostic nanomechanical platforms and introduced diagnostic assays in the field of genomics, protoeomics and microbiomics [1-3]. The nanomechanical detection of biomolecular interactions allows a non-invasive, rapid and personalized diagnosis using nanomechanical cantilever sensors. Specific binding of targets to the cantilever surface induces physical changes in the resonance frequency during mass uptake of the sensor. This is detected by monitoring the position of a laser that reflects from the sensors surface or by tracking the oscillatory frequency of the sensors. Internal reference sensors negate environmental and nonspecific effects. The oscillation mechanics of the sensor has two key parameters the intrinsic mass and the spring constant of the single-clamped beams.

The individual functionalization of sensors with capillaries or ink-jet spotting provides a means to facilitate differential mass uptake in subsequent experiments. Surface stress between the top and bottom surface due to steric hindrance during hybridisation and electrostatic repulsion between neighbouring surface bound molecules could affect the spring constant during the measurement. The repulsion within the layers can be manipulated by changing the ionic strength in the surrounding solution.

In this project, we will investigate the possibility to change the spring constant and the mass while being mounted in the diagnostic chamber. We will pattern the surface functional interface and evaluate the mechanics of such sensors for subsequent quantitative analytics. We will use state of the art cantilever array sensing devices to characterize the assays.

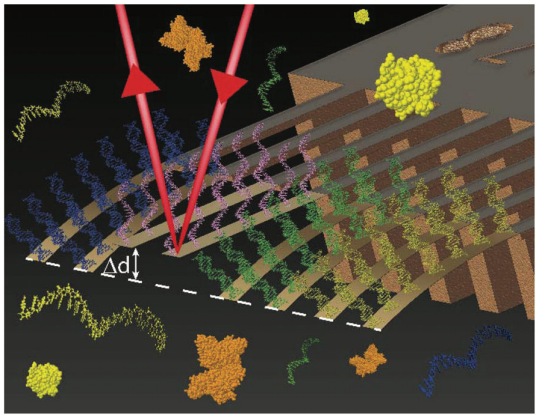



Illustration of nucleic acids target binding on the nanomechanical cantilever array surface.

(1) Brunetti, G., De Pastina, A. and Hegner, M. (2021) Nanoscale Advances 3, 6903–6911
(2) J. Duffy, F. Padovani, G. Brunetti, P. Noy, U. Certa and M. Hegner **Nanoscale**, (2018) 10, 12797
(3) G. Brunetti, et al **Microelectronic Engineering 287 (2024) 112154**

**School of Physics Senior Sophister Research Project 2026**

# Targeted in-situ biofunctionalization of nanomechanical sensors for the recognition of biomolecular interactions

**Prof. Martin Hegner**
**hegnerm@tcd.ie**

The Hegner Group pioneered the development of label-free biomolecular diagnostic nanomechanical platforms and introduced diagnostic assays in the field of genomics, protoeomics and microbiomics [1-3]. The nanomechanical detection of biomolecular interactions allows a non-invasive, rapid and personalized diagnosis using nanomechanical cantilever sensors. Specific functionalization of cantilever surface enables mass uptake of biological targets on the sensors, which is detected by tracking the oscillatory frequency of the sensors. Internal reference sensors negate environmental and nonspecific effects.

The individual functionalization of sensors with capillaries or ink-jet spotting provides a means to detect differential specific binding of biomolecular targets. We performed cantilever array experiments that explored the differential detection of malaria parasites or SARS CoV2 variants of concern in serum simultaneously.

In this project, we will investigate the possibility to address the *in situ* functionalization of cantilever surfaces with nucleic acid tagged receptors while being mounted in the diagnostic chamber analyze the quantitative binding and evaluate the regeneration of such interfaces for subsequent analytical samples. We will use state of the art cantilever array sensing devices and scanning probe microscopy to characterize the assays.

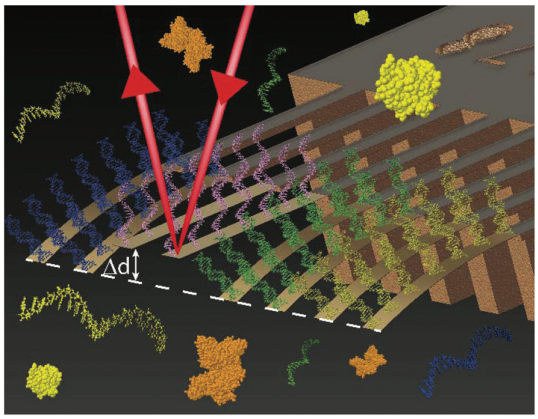



Illustration of nucleic acids target binding on the nanomechanical cantilever array surface.

(1) J. Zhang, H.-P. Lang, F. Huber, A. Bietsch, W. Grange, U. Certa, R. McKendry, H.-J. Güntherodt, M. Hegner and C. Gerber, Nature Nanotechnol. (2006) 1, 214–220.
(2) J. Duffy, F. Padovani, G. Brunetti, P. Noy, U. Certa and M. Hegner **Nanoscale**, (2018) 10, 12797
(3) G. Brunetti, F. Padovani, A. De Pastina, C. Rotella, A. Monahan, S. Hoffman, S. Jongo, S. Abdulla, G. Corradin, G. Pluschke, C. Daubenberger, and M. Hegner **Nanoscale** (2021) DOI: 10.1039/D0NR08083G

## Design and Simulation of Cryogenic Sample Shield Performance

Prof. Lewys Jones & Dr Jon Peters, Ultramicroscopy Research Group

(www.tcd.ie/Physics/research/groups/ultramicroscopy/)

**Keywords:**

Cryogenic electron microscopy, thermal modelling, mechanical design.

**Abstract:**

Electron microscopes use a beam of accelerated electrons as their illumination rather than visible light. As a result, they can achieve far greater magnifications and resolutions down to the atomic scale. The transmission electron microscope is a crucial technology in the study of single protein molecules, often studying these as cryogenically frozen aqueous suspensions. These must be kept deeply frozen during imaging (≈ -170°C), but at the same time protected from unwanted ice build-up from residual moisture in the vacuum chamber (condensing and freezing to the specimen). This unwanted ice build-up causes the samples to become thicker and strongly degrades imaging performance.

In a cryo-EM lens, there is a small gap where the sample sits, Figure 1 [1].

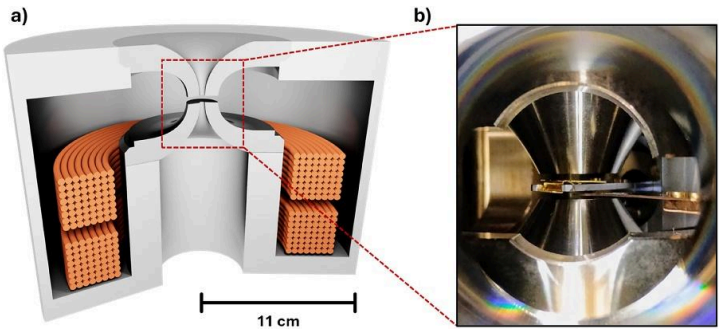



*Figure 1. Schematic of a TEM objective lens showing the sample inserted in-between the pole-piece gap [1].*

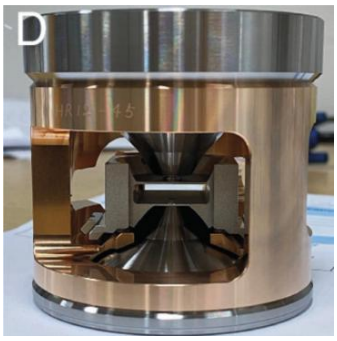


*Figure 2. A variant of a TEM pole-piece with a 'cryo box' (central rectangular opening) that shields the specimen from heat and vacuum residual moisture [2].*

The sample is then shielded from the vacuum moisture by a 'cryo box', Figure 2, which collects water ice instead of the specimen. The goal of this work is to model the heat flow to this cryogenic box as well as the ballistic movement of low-pressure water molecules, and to refine the design of future cryo-shields.

**Expected Outcomes:**

During this project, with the support of others in the research group, the student will:

- Learn the basics of 3D drawing using SolidWorks software,
- Model heat-flows using the COMSOL simulation package,
- Identify pinch-points to the heat-flow or deficiencies in the cryo-shield geometry,
- Propose refinments for the cryo-shield and model these, and
- 3D print a plastic model of the proposed improvements for review.

**Further Details:**

The project and desk will be based in the Advanced Microscopy Laboratory (www.tcd.ie/crann/aml). The ideal student will have an interest in programming, image analysis, and computing. Experience with programming is strongly preferred.

**References:**

[1] Motta Alves, G., Andrews, T., McBean, P., Wells, T., El-Gomati, M., Burkhalter, S., Schulze-Briese, C., Zambon, P., McMullan, G., Henderson, R., Russo, C. and Jones, L. (2025), *"The Dublin lens: a Cc = 1.0 mm objective lens intended for CryoEM at 100 keV"*. Methods in Microscopy. https://doi.org/10.1515/mim-2025-0019

[2] McMullan, G. et al., (2023), *"Structure determination by cryoEM at 100 keV"*. Proceedings of the National Academy of Sciences of the United States of America, 120(49), e2312905120. https://doi.org/10.1073/pnas.2312905120

**Dielectric metasurfaces for emission enhancement**

Supervisor: Prof. Louise Bradley

Optical metasurfaces are surfaces of nanostructured elements which provide for unprecedent control of the optical properties of reflection and transmission of light as well as the light-matter interaction[1, 2]. High refractive index metasurfaces provide for regions of strong electric field enhancement. $TiO_2$ has a relatively high refractive index with n>2[3]. Meta-atoms with broken symmetry had can support resonances called bound states in the continuum as a route to achieving high field enhancement, confinement and high quality factors[4]. This field enhancement has been shown to be of benefit for bulk and surface sensing applications[5].

An example of a tilted ellipse $TiO_2$ metasurface is shown the figure. It has been observed that the QDs dispersed on the metasurface show a highly polarization dependent emission enhancement.. The conditions to optimise the enhancement will be investigated through design, fabrication and characterization of the metasurfaces, with and without the QDs on the surface. The design will be carried out using a commercial finite difference time domain simulation tool. The fabrication requires a combination of electron beam lithography and reactive ion etching. The optical characterization will include reflectance, transmittance, photoluminescence and time-resolved photoluminescence measurements.

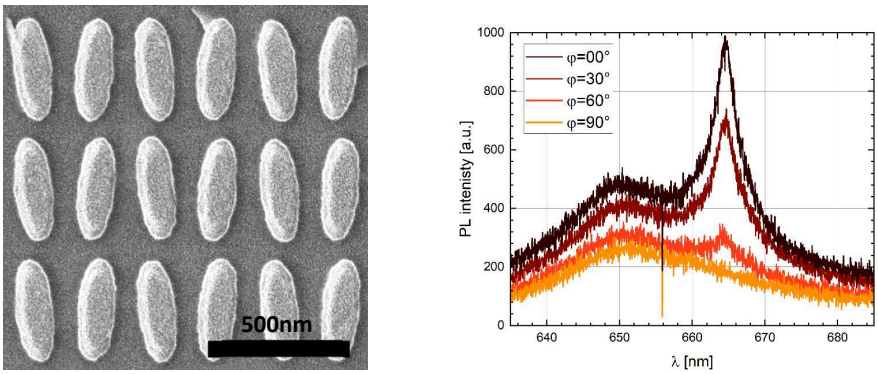



Figure 1: (lhs) A scanning electron micrograph image of a $TiO_2$ metasurface. (rhs) The polarization dependent QD emission showing a large enhancement at the resonance wavelength of the quasi-bound state in the continuum mode.

(1) Koshelev, K.; Kivshar, Y. Dielectric Resonant Metaphotonics. *ACS Photonics* **2020**, *8* (1), 102-112. DOI: 10.1021/acsphotonics.0c01315.
(2) Koshelev, K.; Lepeshov, S.; Liu, M.; Bogdanov, A.; Kivshar, Y. Asymmetric Metasurfaces with High-Q Resonances Governed by Bound States in the Continuum. *Physical Review Letters* **2018**, *121*, 193903. DOI: 10.1103/PhysRevLett.121.193903.
(3) Zhang, X.; Lawless, J.; Li, J.; Peters, L.; McEvoy, N.; Donegan, J. F.; Bradley, A. L. Absorbance Enhancement of Monolayer MoS2 in a Perfect Absorbing System. *Physical Review Materials* **2022**, *6*. DOI: 10.1103/PhysRevMaterials.6.045202.
(4) Zhang, X.; Bradley, A. L. Polaritonic critical coupling in a hybrid quasibound states in the continuum cavity–WS2 monolayer system. *Physical Review B* **2022**, *105* (16). DOI: 10.1103/physrevb.105.165424.

**Coupling a single quantum dot with a single plasmonic nanocavity as a route to single photon emission for quantum applications**

Supervisor: Prof. Louise Bradley

The interaction between quantum emitters and plasmonic nanostructures is a central topic in nanophotonics, with significant implications for quantum optics and photonic device engineering. Quantum dots (QDs) are semiconductor nanocrystals that can act as single-photon sources due to their discrete energy levels and size-tunable emission. Gold bipyramids (BPs) are a class of plasmonic nanoparticles known for their sharp tips and strong localized surface plasmon resonances, which can generate intense electromagnetic near-fields. When a QD is positioned in close proximity to a BP, the local density of optical states experienced by the QD is modified. This can lead to either enhancement or quenching of the QD's spontaneous emission rate, depending on the spatial arrangement and spectral overlap between the QD emission and the BP plasmon resonance.

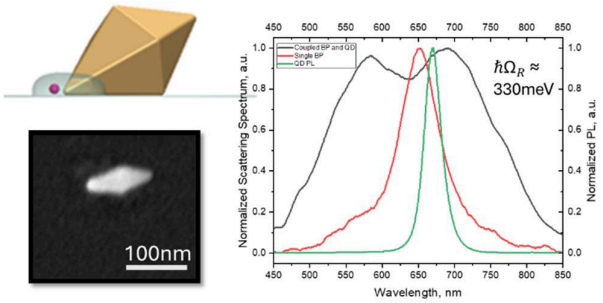



Figure: (top left) Schematic of the coupled QD-Au BP, (bottom left) scanning electron micrograph image of a single Au bipyramid and (right) dark-field scattering spectra of a single Au BP and a coupled QD-Au BP system, as well as the emission spectrum of the QD.

The primary objective of this project is to investigate the emission properties of a single QD coupled to a single gold BP nanoresonator, using a combination of finite-difference time-domain (FDTD) simulations and experimental characterization. A schematic of the structure is shown in the figure along with spectral evidence of the strong coupling of the QD and Au bipyramid resonances. The project aims to understand and control the conditions under which emission enhancement or quenching occurs, with the broader goal of optimizing these hybrid systems for single-photon source applications. Specifically, the project will involve aspects of simulation and experimental characterization. The emphasis on one or the other can be adapted based on the student's preferences.

***Numerical Simulations***

Building on the existing 3D FDTD model for scattering and absorption, we will implement a dipole emitter at the quantum dot's position—matching its photoluminescence wavelength—to simulate and analyse emission properties in the presence of the gold bipyramid nanoresonator.

***Optical Characterization***

Use single-particle spectroscopy to measure the spectral properties and photon statistics of individual BP-QD pairs.

Investigate the influence of BP geometry and QD placement on emission behaviour.

**Strong light-matter coupling using plasmonic Au bowtie nanoantennas**

Supervisor: Prof. Louise Bradley

Light-matter interaction can occur different regimes, including weak, strong and extreme strong coupling. Plasmonic nanostructures provide for sub-diffraction limited localisation of the optical field and large field enhancement with this every small mode volume. These are two of the pre-requisites to achieve strong coupling at room temperatures. In the weakly coupled regime when the plasmon mode is resonant with the exciton mode of a nanoscale emitter only a single peak is visible in the absorbance and emission spectra. However, in the strong coupling regime this splits into two peaks, which never cross, the upper and lower polariton branches. These correspond to the new fundamental states of the systems which are half-plasmon and half-exciton. Energy is coherently exchanged between the exciton and the plasmon[1-3].

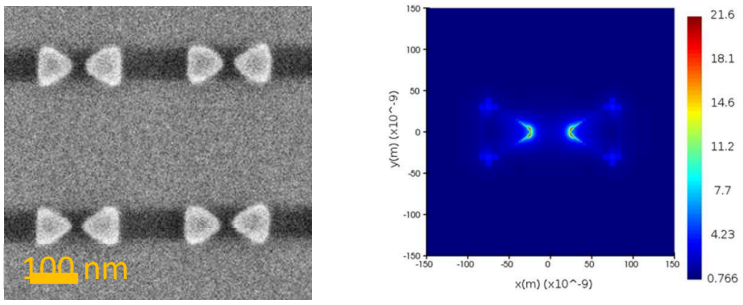



Figure: (left) Scanning electron microscopy image of the Au bowties. (right) Colour-map of the electric field enhancement in the Au bowtie structure.

As shown in the figure Au bowtie nanoantennae with edge lengths of 60 nm and gaps of <40 nm have been fabricated. Such structures show a 20-fold enhancement of the electric field at tips of the bowties, which corresponds to a 400-fold increase in the light intensity in the gap of the bowtie. This project will investigate if such structures can achieve strong coupling at room temperature with different types of nanoscale emitters including single QDs and monolayer $WS_2$. The initial part of the project will use numerical simulations of the structures to determine which system is most suitable for emission in the strong coupling regime. In the second phase of the project the optimum emitter will be selected, and the structures will be fabricated and characterised. The simulations will be carried out using Lumerical, a commercial finite different time domain tool. It will be used to investigate the systems in the frequency and time domains to observe the spectral splitting, the coherent energy exchange and to investigate the emission properties. It will also be used to consider how the plasmonic resonator geometry and environment of the nanoscale emitter can be modified to increase the polariton emission.

(1) Li, J.-Y.; Li, W.; Liu, J.; Zhong, J.; Liu, R.; Chen, H.; Wang, X.-H. Room-Temperature Strong Coupling Between a Single Quantum Dot and a Single Plasmonic Nanoparticle. *Nano Letters* **2022**, *22* (12), 4686-4693. DOI: 10.1021/acs.nanolett.2c00606.
(2) Liu, R.; Zhou, Z. K.; Yu, Y. C.; Zhang, T.; Wang, H.; Liu, G.; Wei, Y.; Chen, H.; Wang, X. H. Strong Light–Matter Interaction in Au Nanorod–Quantum Dot Coupled Systems. *Phys. Rev. Lett.* **2017**, *118*, 237401.
(3) Lu, Z.; Song, D.; Lin, C.; Zhang, H.; Zhang, S.; Xu, H. Plexciton Photoluminescence in Strongly Coupled 2D Semiconductor–Plasmonic Nanocavity Hybrid. *ACS Nano* **2025**, *19*, 5637.

## Experiments with dripping high viscosity liquids

Stefan Hutzler, stefan.hutzler@tcd.ie

The Fitzgerald library hosts a case containing a funnel filled with a very viscous black substance. In fact, it is so viscous that it takes about 10 years for a single drop to detach from it. How can one determine the viscosity of such a drop? Is it possible to determine its surface tension from an analysis of its shape?

This project entails data analysis for the Trinity tar drop, as well as experiments with honey, and with a replicate of the Trinity drop, recently sent out to schools all over Ireland, with a drop time of about 3 months.

**References:**

Bergin, S.D., Hutzler, S. and Weaire, D., 2014. The drop heard round the world. *Physics World*, ***27***(05), pp.26-29. https://doi.org/10.1088/2058-7058/27/05/38

Hutzler, S. and Bradley, L., 2025. Slow science, fast success. *Physics World*, **38**(11), pp.56-56. https://doi.org/10.1088/2058-7058/38/11/31

Hutzler S, Ryan-Purcell JFC, Dunne FF, Weaire D (2018), A simple formula for the estimation of surface tension from two length measurements for a sessile or pendant drop, Philosophical Magazine Letters **98** 9-16.

## The dynamics of structural transitions in ordered foams

Stefan Hutzler, stefan.hutzler@tcd.ie

This experimental project explores the structural transformations of crystalline foam structures. The foams are produced by releasing equal-volume bubbles into cylinders where they spontaneously order into crystalline arrangements. Releasing surfactant solution into such a “columnar crystal” can lead to a rearrangement into a different structure. This project will examine the dynamics of the restructuring using video imaging.

**References:**

Tobin ST, Barry JD, Meagher AJ, Bulfin B, O'Rathaille CE and Hutzler S (2011), Ordered polyhedral foams in tubes with circular, triangular and square cross-section, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **382**, 24-31.

## Using statistical methods from econophysics to analyze bubble motion in a two-dimensional foam

Stefan Hutzler, stefan.hutzler@tcd.ie

Liquid foams naturally undergo a process known as coarsening, whereby large bubbles grow in time and small bubbles shrink, driven by the diffusion of gas between contacting bubbles. As a consequence, bubbles perform random movements. This project addresses the underlying statistics of these movements, which turns out to be non-Brownian. It rather features non-Gaussian, fat-tailed distributions, similar to what is found in the fluctuation of stock markes. In foams, this is the consequence of structural rearrangements, as cell edges shrink to zero, or small bubbles disappear entirely due to coarsening.

Aim of the project is to analyze comprehensive data sets that are available from numerical simulations of two-dimensional foams (as can be approximated experimentally by squeezing bubbles between two flat glass plates and viewing them from top). This requires the writing/editing of Python code that allows for the computation in the change of bubble positions (similar to “returns” in finance), and then an evaluation of distribution functions of these returns. How can these functions be described mathematically? What are their scaling properties? Further analysis concerns the computation of autocorrelation functions and generalised diffusion coefficients.

**References:**

Denis Weaire and Stefan Hutzler. The Physics of Foams, Oxford University Press, 1999.

Peter Richmond, Jürgen Mimkes, and Stefan Hutzler, Econophysics and Physical Economics, Oxford University Press, 2013.

Richmond, P., Sexton, M.B., Hardiman, S.J. and Hutzler, S., 2014. Generalised diffusion model of asset price fluctuations. *The European Physical Journal B*, *87*(3), p.63.

**School of Physics Senior Sophister Research Project 2026**

# The shape of sessile droplets

**Prof. Matthias Möbius**
**mobiusm@tcd.ie**

The shape of sessile droplets on surfaces is important in applications such as printed electronics, medicine and crop spraying. The shape of a sessile droplet (Fig.1) is determined by the wetting properties (contact angle), surface tension and gravity. For droplets smaller than the capillary length, gravity is negligible and the droplet shape is a spherical cap. However, for larger droplets, gravity flattens the droplet and deviates from the spherical shape. In this project you will determine the droplet shape using analytical and numerical techniques for a wide range of droplet sizes for both hydrophilic and hydrophobic surfaces. The project requires good knowledge of either Python or Matlab.

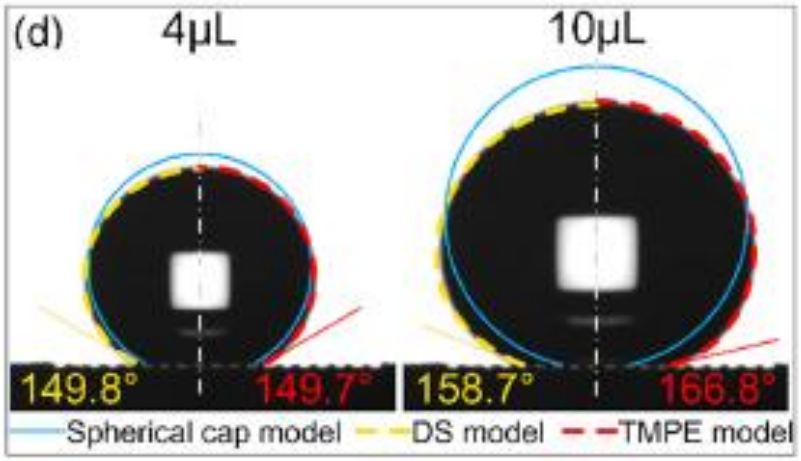



*Figure 1: Water droplets on superhydrophobic surface. The shape is fitted with three different models. The shape of the larger droplet on the right deviates significantly from the spherical cap model as gravity flattens the droplet. Image taken from Hou et al. Colloids and Surfaces A: Physicochemical and Engineering Aspects 656 (2023) 130203.*

**School of Physics Senior Sophister Research Project 2026**

# Ostwald ripening of evaporating breath figures

**Prof. Matthias Möbius**
**mobiusm@tcd.ie**

The collective evaporation of micron sized droplets are relevant in many phenomena such as cloud formation and transmission of pathogens through breath. Here you will study the evolution of micron-sized droplets on a surface during evaporation (see Fig.1). Initially, they undergo Ostwald ripening – larger droplets grow while smaller droplets shrink. It has recently been suggested [1] that this due to differences in vapour concentration above small and large droplets due to the Kelvin effect which states that the vapour pressure is dependent on the curvature of the droplet surface. You will study this effect by measuring the evolution of droplet growth and shrinkage for hydrophobic and hydrophilic surfaces. How do the different wetting properties, which affect the curvature of the sessile droplets, influence the Ostwald ripening process? This is an experimental project but also requires some image processing with ImageJ and/or Python.

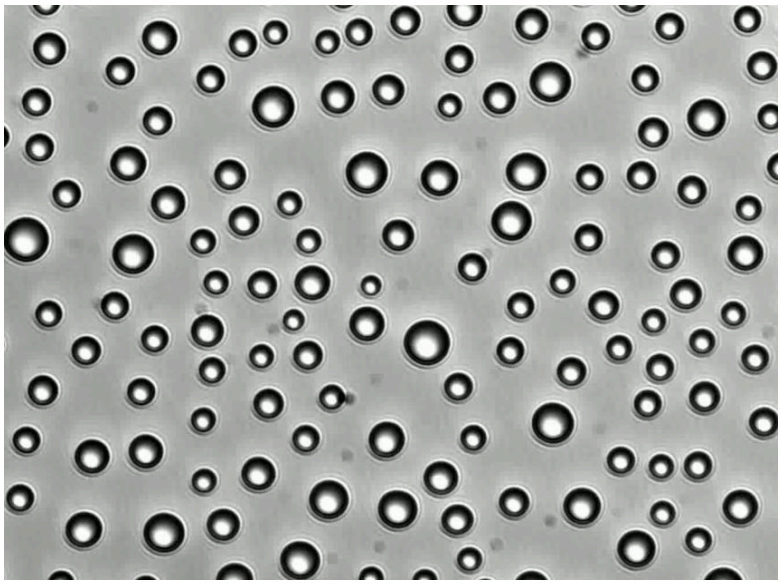


*Figure 1: Micron-sized water droplets on a hydrophobic petri dish formed by breathing on it. The droplets experience Ostwald ripening – smaller drops become smaller while larger drops grow.*

[1] Kilbride, J.J. et al., "Ostwald ripening in evaporating respiratory breath figures", Phys.Rev.Fluids, **10**, L101601 (2025)

**Modelling of Electroencephalography (EEG) Signal Propagation Using Quantum Materials**
Prof Ortwin Hess / Dr Illya Tarasenko

Integrating theoretical simulations with collaborative experimental validation, this project offers students comprehensive training in physics modeling and interdisciplinary collaboration. Outcomes will significantly advance understanding of quantum-material-based electrode performance, directly impacting future developments in EEG technology, neuroscience research, and biomedical device innovation.

**Motivation.** Exploring the interactions of quantum materials with flexible substrates, such as skin, provides essential insights for developing advanced wearable technologies in biomedical and consumer electronics. This project focuses on combining theoretical modelling and simulations with the opportunity to link these predictions to experimental studies conducted by local and international collaborators. Such an integrated approach will significantly enhance understanding of electroencephalography (EEG) signal propagation, optimize electrode configurations, and contribute broadly to the advancement of neuroscience and wearable medical technologies.

**Theoretical and Computational Modelling.** Students will undertake theoretical modelling and simulations using COMSOL Multiphysics software. The modelling will involve creating a simplified representation of EEG signal propagation, starting with basic geometric setups, such as planar dipoles within multilayered media that approximate human biological tissues. Emphasis will be placed on integrating quantum materials, including graphene-based electrodes, into these simulations to investigate potential improvements in EEG signal detection, focusing on enhanced conductivity, signal amplification, and noise reduction.

**Potential Collaborative Experimental Validation.** Although this project is primarily theoretical, students will have opportunities to link their simulation results with practical experiments conducted by local or international neuroscience research groups. These experimental setups typically involve using agar-based substrates to emulate biological tissue properties, embedding dipoles to simulate neuronal sources, and employing quantum-material electrodes to record EEG-like signals.

**Comparative Analysis and Collaboration.** An important potential opportunity of the project will be a comparative analysis between computational simulations and available experimental data provided by collaborators. Students will:

- Compare simulated EEG signals with empirical data, assessing the accuracy and limitations of theoretical models.
- Evaluate and refine computational approaches based on experimental feedback and insights from collaborative researchers.
- Investigate and document the impact of quantum materials in practical EEG scenarios compared to traditional electrodes, with particular attention to signal quality enhancements.

**School of Physics Senior Sophister Research Project 2026**

# Torricelli's law in the viscous limit

**Prof. Matthias Möbius**
**mobiusm@tcd.ie**

Torricelli's law from 1643 is one of the oldest laws in physics and states that the flow velocity out of an orifice is $\sqrt{2gh}$, where $h$ is the height of the fluid level above the orifice [1]. This is the same velocity as an object would attain in free fall from height $h$. However, this only holds for low viscosity fluids such as water where viscous effects are negligible. In this project you will explore how the flow velocity changes as the viscosity of the fluid is increased. How strongly do viscous fluids deviate from this law? This is an experimental project where you will monitor the flow of different fluids with a camera. It will also involve some image processing.

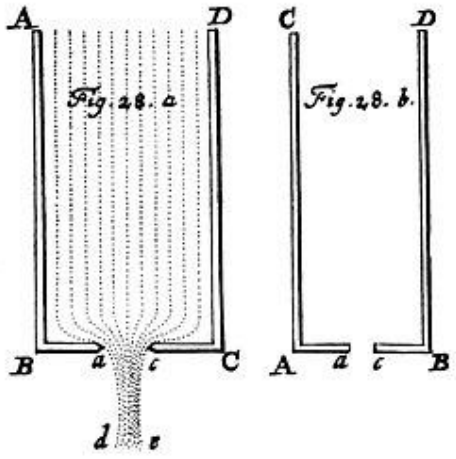



*Figure 1: Sketch of flow from an orifice with streamlines from Daniel Bernoulli's "Hydrodynamica" (1738).*

[1] C. Clanet, "Clepsydrae, from Galilei to Torricelli", Physics of Fluids 12, 2743–2751 (2000).

**Project with the Quantum Theory of Materials Group and Prof. D. O'Regan**

**Email** david.o.regan@tcd.ie **Web** https://theoryofmaterials.com

**1. Accurate modelling of diamond structure semiconductor band gaps**

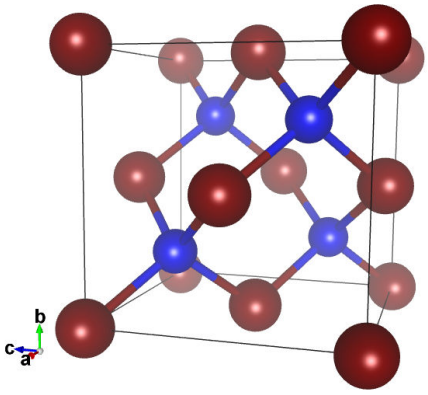



*Figure 1: A unit cell of the GaAs crystal lattice, used for DFT simulations*

The accurate modelling of semiconductor properties can be highly useful for applications such as predicting defect concentrations in solar cell materials. Density functional theory (DFT) technology can model these materials without significantly high computational costs, but the resulting predicted bandgaps are drastically underestimated.[1]

Recent research on transition metal oxides have shown that this underestimation can be reduced at low computational cost with the use of "DFT+U+J" energy corrections based on orbital occupancy numbers.[2-4] It would be interesting to see if this methodology can successfully be applied to non-oxide semiconductor materials.

This project will involve using the procedure described in Refs.[2-4] to determine the correction magnitudes for a number of materials with diamond or zinc-blende lattice, such as Silicon and GaAs. We will then apply these corrections to investigate, e.g. band-structures. These calculations will be performed using high performance computing, but no real programming will be involved. If successful, the project could be a nice demonstration of a method normally used for oxides being useful outside of that domain.

1. Himmetoglu, B.; Floris, A.; De Gironcoli, S.; Cococcioni, M., Hubbard-Corrected Dft Energy Functionals: The LDA+U Description of Correlated Systems. *International Journal of Quantum Chemistry* **2014**, *114*, 14-49.

2. Linscott, E. B.; Cole, D. J.; Payne, M. C.; O'Regan, D. D., Role of Spin in the Calculation of Hubbard U and Hund's J Parameters from First Principles. *Physical Review B* **2018**, *98*, 235157.

3. Orhan, O. K.; O'Regan, D. D., First-Principles Hubbard U and Hund's J Corrected Approximate Density Functional Theory Predicts an Accurate Fundamental Gap in Rutile and Anatase TiO2. *Physical Review B* **2020**, *101*, 245137.

4. Lambert, D. S.; O'Regan, D. D., DFT+U+J with linear response parameters predicts non-magnetic oxide band gaps with hybrid-functional accuracy. *Phys. Rev. Research* **2023**, *5,* 013160.

Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

# Belief Propagation for Quantum Dynamics

**Supervisor**.
Prof. Pieter Claeys (claeysp@tcd.ie)

**Project aim and abstract.**
The dynamical behavior of quantum many-body systems, as probed in a wide range of quantum computing experiments, is notoriously difficult to simulate using classical algorithms. Tensor networks are one of the most widely used approaches to study this problem numerically, and have recently been combined with belief propagation to accurately simulate cutting-edge experiments on quantum dynamics [1-3]. This project aims to relate “loop corrections” in belief propagation to memory effects in quantum dynamics.

Starting from perfectly Markovian quantum dynamics in minimal quantum circuits [4], in which belief propagation can be applied without any approximation, non-Markovian effects can be systematically reintroduced, for which an accurate approximation requires belief propagation to be supplemented by cluster (loop) corrections. Following a successful implementation of the Markovian dynamics in a minimal model, this project aims to quantify both the accuracy and the breakdown of such corrections and use these to obtain physical insights in the role of non-Markovianity in quantum systems.

**Research methods.**
This project is largely numerical, based on tensor network simulations using Python or Julia, with an additional theoretical component based on the student’s interest using graphical techniques in quantum circuits.

**References.**
[1] R. Orus, Annals of Physics 349, 117-158 (2014)
[2] J. Tindall *et al.*, Physical Review X Quantum 5, 010308 (2024)
[3] S. Midha *et al.*, arXiv:2604.03228 (2026)
[4] Bertini *et al.*, Review of Modern Physics 98, 025001 (2026)

**Project Title:** *Localisation suppression in low-dimensional quantum systems with correlated disorder*

**Supervisor**: Mauro Ferreira

**Description:** A well-known feature of low-dimensional quantum materials is that charge transport is extremely sensitive to disorder: even a minute amount of uncorrelated impurities can localise electronic wavefunctions and strongly suppress conductance. However, not all disorder acts in the same way. When correlations are present (through quasiperiodic potentials or structured impurity configurations) this conventional picture can break down, allowing robust conduction to persist or even re-emerge. In this project, the student will investigate how different forms of disorder affect quantum transport in one-dimensional systems, focusing on paradigmatic models such as the Anderson and Aubry–André–Harper chains [1,2]. Using numerical techniques based on Green's functions and quantum transport theory, the project will explore regimes in which impurities that normally act as strong scatterers become effectively "invisible", leaving the electronic current unaffected [3,4]. The work highlights how correlated disorder can suppress localisation and provides insight into strategies for engineering and controlling conductivity in nanoscale quantum materials.

Bibliography:

[1] "*Inverse determination of light-matter coupling in disordered systems from transmittance spectra*", https://doi.org/10.48550/arXiv.2511.12647

[2] "*Multifractal critical phase driven by coupling quasiperiodic systems to electromagnetic cavities*", Phys. Rev. B 112, 174202 (2025)

[3] "I*mpurity invisibility in graphene: Symmetry guidelines for the design of efficient sensors*", Phys. Rev. B **94,** 045417 (2016)

[4] "*Effective Delocalization in the One-Dimensional Anderson Model with Stealthy Disorder*", Phys. Rev. Lett. **136**, 150404 (2026)

**Project title:** Crystalline and amorphous structures in 2D systems: a theory perspective
**Supervisor:** Prof. Mauro Ferreira ( ferreirm@tcd.ie )

**Description:** Crystalline structures play a major role in determining the physical properties of materials and for that reason it is paramount to understand how they are formed. While Solid State Physics describes and explains how atoms and molecules spontaneously crystallise, it is not so clear how classical objects self-assemble into ordered structures in macroscopic systems, especially when the mutual interaction between such objects differs from the usual force fields seen in the nanoscale. Motivated by an old experimental set up that creates such ordered structures with a cluster of classical objects, the question that this project addresses is under what conditions a given crystalline structure is more favourable than another. Likewise, what is the impact that the introduction of one or more defects may bring to such structures? While these are questions that such an experimental setup can address, there is very little theory done with these systems. The goal of the current project is to develop a simple modelling tool capable of predicting the most favourable structure a collection of classical objects will spontaneously adopt. This tool can be put to the test with experimental measurements that will be carried out during the course of the project [1,2]. The project calls for a solid background in Physics and Mathematics as well as good coding skills. Quantum Mechanics and Solid State Physics plays a major part in the project and students will have the opportunity to improve and develop their knowledge on these two subjects.

REFERENCES:

[1] P. D S. Lima, A. Lyons, A. Irannezhad, J. M. de Araújo, Stefan Hutzler and M. S. Ferreira, "*Self-assembled clusters of magnetically tilted dipoles*", Phys. Rev. E **110**, 064134 (2024)

[2] P. D. S. de Lima, R. De La Cour, K. Gaff, J. M. de Araújo, S. J. Cox, **M.S. Ferreira** and S. Hutzler, "*Self-assembled clusters of mutually repelling particles in confinement*", Phys. Rev. E **112**, 044150 (2025)

# Numerical optimization of dissipative preparation protocols for topological states

Mattia Moroder

**Background and motivation** Preparing target many-body quantum states is a central goal of quantum simulation and computation. While most established protocols rely on unitary dynamics, dissipative state preparation (DSP) has emerged as a powerful alternative: by engineering system-environment interactions, one drives an arbitrary initial state toward a desired target as the unique fixed point of a Lindbladian. Compared to unitary schemes, DSP removes the need for a finely tuned initial state, reduces post-selection overheads, and inherits noise resilience from its fixed-point structure [1]. A fundamental open question concerns the limits on preparation time: local Lindbladians obey Lieb-Robinson bounds [2], and gapped Lindbladians necessarily exhibit exponential decay of correlations in the steady state, suggesting an unavoidable interplay between the spatial support of the dissipator and the time needed to prepare long-range correlated states. Recently, exact locality-preparation time tradeoff relations were derived for quadratic systems by exploiting the freedom of mixing Bogoliubov jump operators through a matrix $\mathbf{B}$, restricted to be unitary and to systems with periodic boundary conditions, where analytical results are accessible [3].

**Project goals** This thesis aims to extend that framework numerically by dropping the unitarity constraint on $\mathbf{B}$ and considering arbitrary, full-rank mixing matrices, which preserve the steady state but enlarge the space of admissible dissipators. The student will (i) implement the Kitaev chain with open boundary conditions, whose topological phase hosts edge-localized Majorana zero modes, topologically protected excitations of interest for robust quantum computation; (ii) diagonalize the resulting Lindbladian using the third-quantization formalism to obtain the full spectrum and, in particular, the dissipative gap that controls the asymptotic preparation time; and (iii) use gradient-descent-based optimization of the entries of $\mathbf{B}$ to identify jump operators that are simultaneously as local as possible in real space and as gapped as possible (the preparation time scales as the inverse dissipative gap). The expected outcome is a quantitative map of the achievable tradeoff in the various phases of the model (trivial, topological, and critical) and a comparison with the analytical bounds known in the unitary case.

**Optional extensions** If time allows, the student may explore more sophisticated optimization schemes (e.g., ADAM or other adaptive methods) and extend the approach to further quadratic topological models, such as the Su-Schrieffer-Heeger (SSH) chain.

**Expected impact** A successful completion of this project will provide a concrete numerical methodology for designing optimally local dissipators in topological systems, complementing existing analytical results and paving the way toward efficient experimental realizations of topological states on analog quantum simulation platforms.

## References

[1] Lin Lin. Dissipative preparation of many-body quantum states: Toward practical quantum advantage. *APL Computational Physics*, 1(1):010901, 09 2025. arXiv:https://pubs.aip.org/aip/aco/article-pdf/doi/10.1063/5.0283315/20690373/010901_1_5.0283315.pdf, doi:10.1063/5.0283315.

[2] David Poulin. Lieb-robinson bound and locality for general markovian quantum dynamics. *Phys. Rev. Lett.*, 104:190401, May 2010. URL: https://link.aps.org/doi/10.1103/PhysRevLett.104.190401, doi:10.1103/PhysRevLett.104.190401.

**Learning to Solve Physical Problems using High Performance Computing Methods**

**Project Supervisor Prof. Charles Patterson Charles.Patterson@tcd.ie**

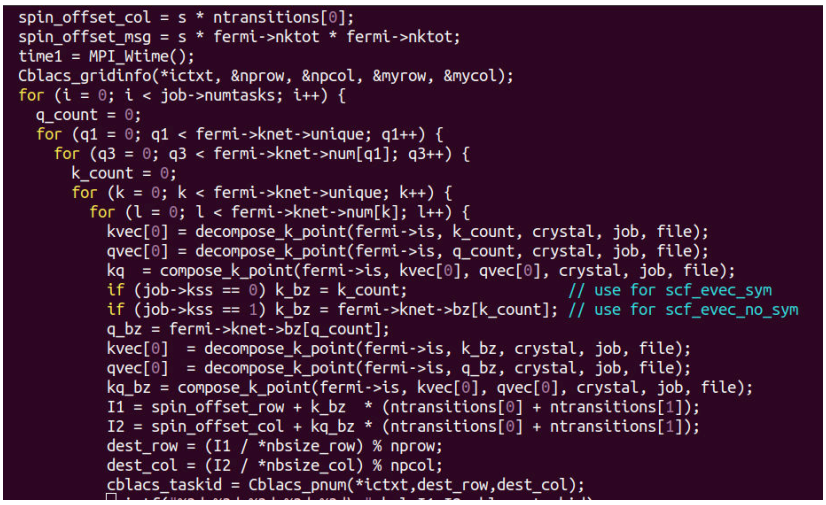
High performance computing (HPC) methods use parallel computing over large numbers of compute cores to solve large problems which are not solvable on single CPU systems. The methods include Message Passing Interface (MPI), multi-threaded computing with OpenMP and architectures such as multicore shared memory systems and graphical processing units (GPUs). There are libraries of software routines such as ScaLAPACK, which is the parallel extension of LAPACK, the Linear Algebra Package. Learning to programme using these systems and libraries requires new ways of thinking compared to serial procedural programming.

MPI [1] is available for Python using the mpi4Py library [2] combining the ease of programming in Python with the power of HPC. mpi4Py can be imported in the same way as NumPy or SciPy, which are the scientific libraries for Python.

OpenMP-like programming [3] is available for Python using Pymp [4].

Serial LAPACK [5] routines are used to solve a wide range of linear algebra problems in scientific computing such as solving systems of linear equations and solving eigenvalue problems. The parallel extension of LAPACK, ScaLAPACK [6], allows large linear algebra problems to be solved.

In this project you will learn to code in some of the methods mentioned above. The problem set could include solution of partial differential equations or another problem mutually agreed with the supervisor.



```
spin_offset_col = s * ntransitions[0];
spin_offset_msg = s * fermi->nktot * fermi->nktot;
time1 = MPI_Wtime();
Cblacs_gridinfo(*ictxt, &nprow, &npcol, &myrow, &mycol);
for (i = 0; i < job->numtasks; i++) {
  q_count = 0;
  for (q1 = 0; q1 < fermi->knet->unique; q1++) {
    for (q3 = 0; q3 < fermi->knet->num[q1]; q3++) {
      k_count = 0;
      for (k = 0; k < fermi->knet->unique; k++) {
        for (l = 0; l < fermi->knet->num[k]; l++) {
          kvec[0] = decompose_k_point(fermi->is, k_count, crystal, job, file);
          qvec[0] = decompose_k_point(fermi->is, q_count, crystal, job, file);
          kq  = compose_k_point(fermi->is, kvec[0], qvec[0], crystal, job, file);
          if (job->kss == 0) k_bz = k_count;                  // use for scf_evec_sym
          if (job->kss == 1) k_bz = fermi->knet->bz[k_count]; // use for scf_evec_no_sym
          q_bz = fermi->knet->bz[q_count];
          kvec[0]  = decompose_k_point(fermi->is, k_bz, crystal, job, file);
          qvec[0]  = decompose_k_point(fermi->is, q_bz, crystal, job, file);
          kq_bz = compose_k_point(fermi->is, kvec[0], qvec[0], crystal, job, file);
          I1 = spin_offset_row + k_bz  * (ntransitions[0] + ntransitions[1]);
          I2 = spin_offset_col + kq_bz * (ntransitions[0] + ntransitions[1]);
          dest_row = (I1 / *nbsize_row) % nprow;
          dest_col = (I2 / *nbsize_col) % npcol;
          cblacs_taskid = Cblacs_pnum(*ictxt,dest_row,dest_col);
```

[1] https://www.mcs.anl.gov/research/projects/mpi/
[2] https://mpi4py.readthedocs.io/en/stable/intro.html
[3] https://www.openmp.org/
[4] https://pymp.readthedocs.io/en/latest/
[5] https://www.netlib.org/lapack/lug/
[6] http://www.netlib.org/scalapack/

**Parameter Optimisation using Linear Least Squares, LASSO and Ridge Regression Methods**

**Supervisor: Prof. Charles Patterson (Charles.Patterson@tcd.ie)**

Fitting a set of {x, y} data pairs to a straight line is perhaps the simplest example of use of the Linear Least Squares method in which the sums of squares of residuals – differences between the model prediction and actual data points – is minimised for a certain value of the slope and intercept. Things get more complex when dealing with the dependence of one variable on multiple other variables. For example, in medicine, how does the risk of a particular disease depend on a set of variables? Which variables are the best predictors of the susceptibility of an individual to a disease? How do you handle cases where some of the variables are strongly correlated?

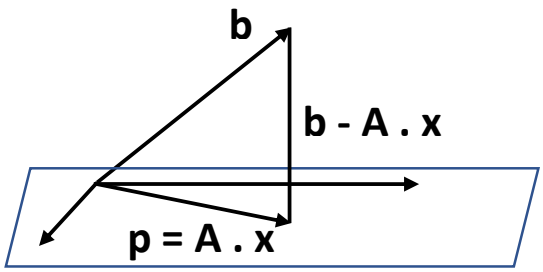



Figure: Linear least squares solution of **A . x = b** by projection onto the column space of **A**.

Statisticians have been thinking about these problems for decades but these questions have come to the fore in the age of machine learning where large data sets are analysed in order to learn how one variable depends on another. How do you optimise a desired outcome by manipulating variables which are under your control, for example, in synthesizing new materials with desired properties? Answers to some of these questions were given by Hoerl and Kennard in the 1970's [1].

You will learn about the trade-off in bias and variance. Optimum fits are obtained using regularisation methods such as Least Absolute Shrinkage and Selection Operator [2] (LASSO) or Ridge Regression [1, 3].

The project will be computational and will use linear algebra methods such as the singular value decomposition (SVD). Together with the project supervisor, you will choose a problem for study after spending some time learning about the methodology.

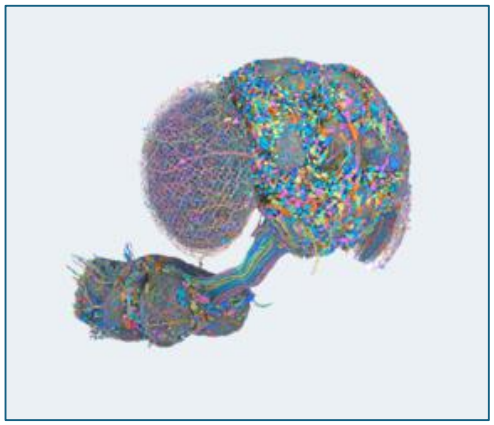
[1] https://www.jstor.org/stable/1271436

[2] https://bookdown.org/tpinto_home/Regularisation/lasso-regression.html

[3] https://www.publichealth.columbia.edu/research/population-health-methods/ridge-regression

**Analysis of a brain connectome**

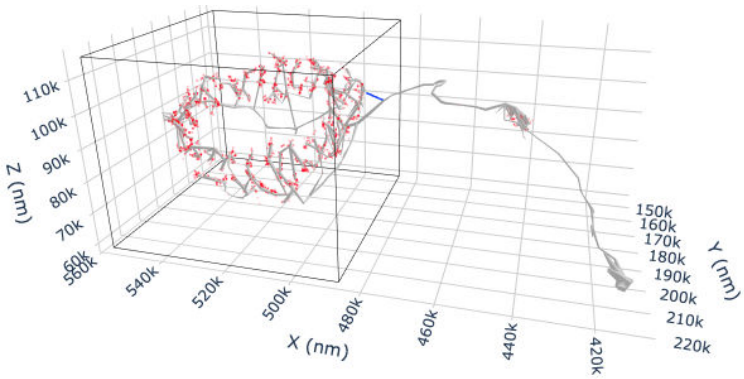
This project will analyse the properties of a whole-brain connectome. The connectome is a comprehensive description of the neural connections in a brain or nervous system. It specifies neurons, synapses, the direction of information flow, the spatial geometry of each neuron, and the network structure formed by all connections. The project will use the connectome of the adult Drosophila (fruit fly), containing approximately 140,000 neurons and 50 million synapses, which was released in June, 2024. It represents the first whole-brain connectome of a complex animal and the first connectome with full 3D meshes for every neuron. Access to the connectome is through a Python API which acts as a client of a cloud-hosted database (FlyWire).



The emphasis of the project will be on the analysis of the suspected critical behaviour that neuronal networks may display to maximize information flow. Possible avenues to explore are:

- Building adjacency matrices from synapse tables
- Track size of largest connected component
- Look for sharp transitions in connectivity
- Extraction of exponents to compare with values observed in Very Large Scale Integrated (VLSI) digital circuits

An example of the type of analysis that can be constructed using the Python API is shown on the right. The box bounds a highly connected region called the Ellipsoidal Body (EB), which is the fly's navigation hub and lies in the center of its brain. This region contains over half a million synapses.




The plot shows just one neuron (grey) and its associated synapses (red) that are contained within the EB. The purpose of the program is to identify the dendritic segments of each neuron that cross the box boundary (crossing segments are shown in blue).

The scope of this project is as follows:

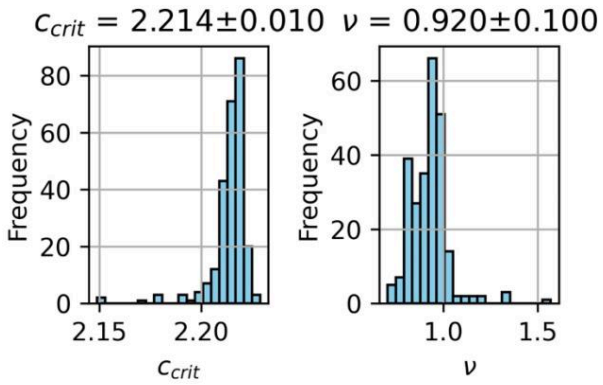
- Understand the structure of the Python API and display dendritic structure
- Explore different regions of the fly brain and select one for further analysis
- Extract statistical data from the selected region so that comparisons with VLSI circuits and critical phenomena can be made.

**Measurement of critical phenomena in very large digital circuits**

Large digital circuits can contain many hundreds of thousands of standard logic cells (including basic NAND and NOR functions, but also more complex flip-flops and multiplexers). The optimization of the placement of these cells to minimise the total length of the wires connecting the cells is critical to ensuring that the circuit's demand for wiring resources can be met by the supply of wiring resources (defined in terms of the number of metal wiring layers and the wiring pitch). If the demand for wiring exceeds the supply (for example, if the number of connections between cell is too high) the circuit is unrouteable, and an expensive redesign is required.

This project interprets the transition from routability to unroutability as the connectivity $c$ between cells increases (interpreted as the average number of cells a cell is connected to) in terms of a critical phase transition. This transition is characterised by a divergence in the average wire length and is associated with a critical connectivity $c_{crit}$ and the transition is approached with a critical exponent $\upsilon$.

Initial experiments using Python-based cell placement optimization algorithms have resulted in the measurement of the critical point at $c_{crit} = 2.21 \pm 0.008$ and an associated critical exponent of $\upsilon = 0.91 \pm 0.08$.




This initial analysis was limited by the relatively small circuit sizes that could be optimized within a reasonable time frame (a single circuit composed of 64,000 cells required a run time of two days). This follow-on project will use a commercial grade Electronic Design Automation (EDA) tool for cell placement optimization, called RePlAce from the OpenRoad consortium. It is anticipated that by using a commercial tool for the design of Very Large Scale Integrated (VLIS) circuits, much larger circuits can be investigated (the hope is circuits with greater than one million cells) and therefore much more accurate estimates of the critical parameters can be made.

This experimental project will run in parallel with a theoretical project and will provide information to guide the theoretical determination of the critical parameters.

The scope of the project is as follows:

- Explore use of RePlAce to optimise benchmark digital circuits
- Design standard cells to be used in critical phase transition experiments using Python
- Synthesis of idealized netlists to be used in critical phase transition experiments using Python
- Extraction of data from optimised circuits of different sizes to infer critical parameters in the infinite size limit.

## Theoretical analysis of critical phase transitions in digital integrated circuits

Large digital circuits can contain many hundreds of thousands of standard logic cells (including basic NAND and NOR function but also more complex flip-flops and multiplexers). The optimization of the placement of these cells to minimise the total length of the wires connecting the cells is critical to ensuring that the circuit's demand for wiring resources can be met by the supply of wiring resources (defined in terms of the number of metal wiring layers and the wiring pitch). If the demand for wiring exceeds the supply (for example, if the number of connections between cell is too high) the circuit is unrouteable, and an expensive redesign is required.

This project interprets the transition from routability to unroutability as the connectivity $c$ between cells increases (interpreted as the average number of cells a cell is connected to) in terms of a critical phase transition. This transition is characterised by a critical connectivity $c_{crit}$ and the transition is approached with a critical exponent $\upsilon$. As with a wide variety of other physical systems exhibiting critical phase transitions, the analysis procedure of choice is the renormalization group.

An initial theoretical analysis of the phenomenon using a majority rule renormalization group transformation has predicted $c_{crit} = 1.51$ and $\upsilon = 1$. The figure below shows the comparison of the renormalization group theory and experimental data obtained from the optimization of idealized cell arrays of size $C$ cells.

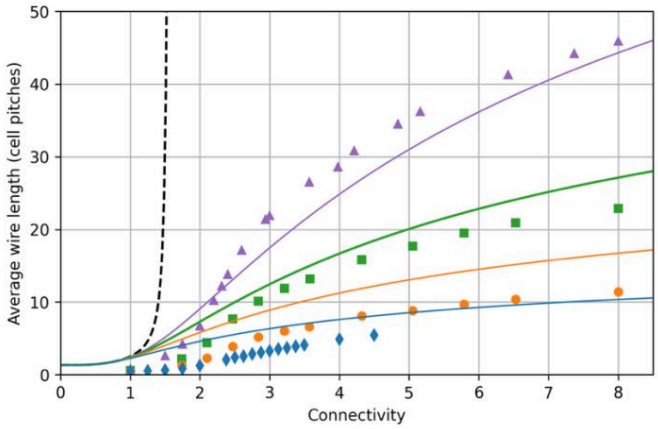



*Figure 1: comparison of theory versus experiment for cell arrays of sizes* $C = 1{,}024\ (blue, diamonds), 4{,}096\ (orange, circles), 16{,}384\ (green,\ squares)$, *65,536 (purple, triangles). For infinite size arrays (dashed line), the predicted theoretical average wire length exhibits a critical point at* $c_{crit} = 1.51$.

The scope of this project is as follows:

- Explore alternative renormalization group transformations to better match the existing experimental data (experimental data suggest at $c_{crit} = 2.21 \pm 0.008$)
- Explore alternative renormalization group transformations which are representative of digital circuit design practice
- Work with a parallel experimental project generating data from much larger cell arrays

# Gibbs Sampling for phase-modulated Neural Quantum States

Artur M. Lacerda

**Background and Motivation.** Neural Quantum States (NQS) provide a variational framework for representing many-body quantum wavefunctions using neural networks. Since the original proposal by Carleo and Troyer [1], NQS have become an important tool for variational Monte Carlo simulations of quantum systems. The original implementation was based on complex-valued Restricted Boltzmann Machines (RBMs), where the wavefunction amplitudes are represented by a complex RBM ansatz.

In classical RBMs, Gibbs sampling is efficient because the model satisfies a conditional independence structure between visible and hidden variables. However, for NQS based on complex-valued RBMs, the sampling probability is given by $|\Psi(\sigma)|^2$. Taking the modulus square of a complex RBM wavefunction destroys the RBM factorization structure. As a consequence, the conditional independence property is lost and Gibbs sampling can no longer be applied directly. These RBM-based NQS implementations therefore rely on Metropolis-Hastings sampling instead.

A phase-separated representation of the wavefunction,

$$\Psi(\sigma) = \sqrt{P(\sigma)}\, e^{i\phi(\sigma)},$$

restores this structure by explicitly representing the probability distribution $P(\sigma)$ with a classical RBM, making Gibbs sampling possible again. Although the field has progressively moved toward deeper neural architectures and autoregressive models, a systematic study evaluating the effectiveness of this approach against standard RBMs and shallow neural-network ansätze is still lacking.

**Project Goals.** The goal of this project is to implement and benchmark a phase-modulated Neural Quantum State ansatz within the NetKet library [2]. The project will compare Gibbs sampling against standard Metropolis sampling in terms of autocorrelation times, sampling efficiency, convergence behavior, and variational accuracy.

The numerical experiments will focus on simple benchmark systems such as the transverse-field Ising model and one-dimensional Heisenberg chains. The project will investigate whether Gibbs sampling can improve the efficiency of variational Monte Carlo simulations while maintaining competitive energy estimates.

**Optional Extensions.** Possible extensions include studying the scaling of autocorrelation times with system size, comparing different phase-network parametrizations, and investigating the behavior of the method in frustrated or two-dimensional systems. Additional comparisons with autoregressive sampling methods may also be considered.

**Expected Impact.** This project aims to provide a systematic evaluation of phase-separated RBM wavefunctions as a practical alternative to standard Metropolis-based Neural Quantum States. The results may clarify whether Gibbs sampling can still offer computational advantages in modern NQS simulations despite the recent focus on deeper architectures and autoregressive approaches.

# Shortcuts to adiabaticity in open quantum systems: purity leakage in dark spaces

Artur M. Lacerda

**Background and motivation.** Shortcuts to adiabaticity (STA) and counterdiabatic protocols are widely used to suppress nonadiabatic excitations in driven quantum systems. Extending these ideas to open quantum systems is considerably more difficult because the dynamics are generated by Lindblad superoperators, so that the corresponding counterdiabatic correction generally becomes a nontrivial superoperator acting on the density matrix. An important exception arises in dissipative systems possessing decoherence-free or dark subspaces (DSs), where the effective counterdiabatic correction can become purely Hamiltonian.

Recent work by Santos, Kamenev, and Gefen [1] studied adiabatic state manipulation in dissipative systems with strong symmetries and dark subspaces stabilized by engineered dissipation. Such protected manifolds are currently of considerable interest in quantum information processing, particularly in dissipative bosonic encodings and cat-qubit architectures. The authors showed that nonadiabatic effects induce decoherence and purity leakage scaling as

$$\Delta\mathcal{P} \sim \frac{1}{\gamma T},$$

where $\gamma$ is the Liouvillian gap and $T$ is the protocol duration. Importantly, the authors explicitly state that this result holds "in the absence of corrective measures", leaving open the possibility that counterdiabatic corrections may suppress leakage outside the instantaneous dark subspace.

**Project goals.** The project aims to reproduce the analytical results of Ref. [1] for the dissipative spin-3/2 model and subsequently investigate corrective protocols designed to suppress nonadiabatic excitations. The student will review the Lindblad formalism for open quantum systems, the structure of decoherence-free subspaces, and the geometric description of adiabatic evolution in dissipative systems.

The project will focus on the time-dependent jump operator introduced in Ref. [1], whose dark subspace evolves through adiabatic rotations of the spin degrees of freedom. The student will derive the effective dark-space dynamics, reproduce the purity-loss scaling predicted in the paper, and analyze the role of the Liouvillian gap in suppressing leakage outside the protected manifold.

The second part of the project will investigate counterdiabatic corrections adapted to the dissipative dark-space setting and study their effect on suppressing nonadiabatic transitions. Corrected and uncorrected protocols will be compared through their purity leakage and fidelity scaling as functions of the protocol duration and Liouvillian gap.

**Optional extensions.** Possible extensions include the implementation of approximate or variational counterdiabatic protocols and considering different dissipative models possessing dark subspaces.

**Expected impact.** The project will provide experience with adiabatic dynamics in open quantum systems and contribute to the study of robust quantum control in dissipative devices. More generally, it will help clarify the role of STA in nonunitary quantum dynamics and their potential application to protected quantum-information architectures based on engineered dissipation.

**School of Physics Senior Sophister Research Project 2026-2027**

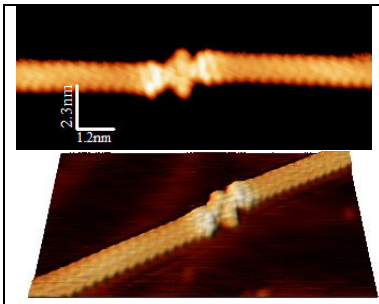
## Simulating interactions and electronic structure of metal-porphyrin nanostructures

**Supervisor: Cormac McGuinness**
**E-mail: Cormac.McGuinness@tcd.ie**
**Materials – Materials – Theory / Computational**

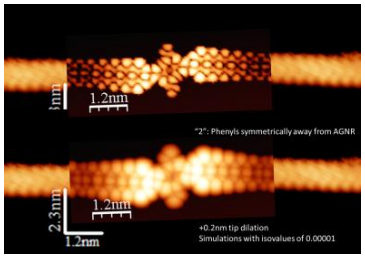
On-surface synthesis (OSS) methods allow for creating entirely novel nanostructures on surfaces derived from precursor molecules rationally designed to form networks. Networks can be constructed from a versatile family of functional molecules – transition metal porphyrins – and further tuned to control the structure of the network. The objective is to simulate and study the electronic structure of porphyrin-derived on-surface synthesized nanostructures/networks.

Porphyrins (Por) are organic molecules with a choice of differing divalent metal ions that can be at the center of their structure (macrocycle) giving differing band-gaps and optical spectra, examples include Fe-Por in heme and Mg-Por in chlorophyll. Porphyrin-derived novel nanostructures or nanonetworks can be formed through on-surface synthesis of halogenated porphyrin precursors resulting in hybrid 1D nanostructures such as in Figure 1(a), or in periodic two-dimensional networks. Figure 1(a) illustrates experimental STM data of a Ni-Por integrated into an armchair graphene nanoribbon (GNR) giving a unique example of a functional GNR (FGNR). Porphyrin functionality is derived especially from the variety of central metal atoms and their interactions or ligation with molecules, illustrated in Fig 1(c).

The project will use appropriate density functional theory (DFT) codes and packages to simulate the electronic structure of either new, existing or proposed porphyrin-derived 2D nanonetworks and 1D nanoribbons. Of particular interest will be the dependence of electronic bandstructure on the central metal, the evaluation of the electronic structure upon ligation or attachment to the central metal of small molecules (e.g. $O_2$, CO, NO) and the simulation of the STM images associated with these interactions. The results obtained will examine band-gaps, densities of states, bandstructure, localisation of the highest occupied (valence band) and lowest unoccupied (conduction band) states and in particular simulations of scanning tunnelling microscopy (STM) images. This will complement our experimental on-surface synthesis inclusive of STM measurements. FHI-AIMS[1] is the most appropriate simulation tool.




(a) Experimental STM image and 3D topographic view of individual FGNR self-assembled on Au(111)




(b) Simulation by DFT of the STM images of an FGNR – a porphyrin incorporated into an armchair graphene nanoribbon.


(c) Illustration of a metal porphyrin unit within a network where the central Fe atom, interacts or ligates with molecular oxygen, as in heme. Simulations of STM of these nanostructures and similar interactions are the goal.

Figure 1: illustrative experimental data (a); simulations of STM by DFT methods (b); and goal (c).

Prior experience with unix/linux, python programming as well as some scripting ability is very useful, but further experience will be gained in these areas. Instead of FHI-AIMS we may explore new workflows using a web+python framework called Aiidalab[2].

[1] Blum V et al "*Ab initio molecular simulations with numeric atom-centered orbitals*" Comput. Phys. Commun., **180** 2175–96, 2009; https://fhi-aims.org

[2] Yakutovich A V. et al "*AiiDAlab – an ecosystem for developing, executing, and sharing scientific workflows*" Comput. Mater. Sci., **188** 110165, 2021

# Efficient qubit reset beyond the Born-Markov approximation

Paul Eastham,
Quantum Light and Matter Group
https://www.tcd.ie/physics/research/groups/qlamg/ easthamp@tcd.ie

One of the fundamental requirements in quantum computing is the ability to reset a quantum bit — a qubit – into a known state. This process requires allowing the qubit to interact with a macroscopic environment, forming a heat bath to which entropy is transferred. In the past it has not been possible to compute dynamics of such a system, comprising a qubit coupled to a macroscopic environment, due to the enormous Hilbert space of the latter. Although approximations, such as the so-called Born-Markov approximation, can be used to produce tractable theories, they are becoming increasingly inaccurate in comparison to the experimental state-of-the-art.

Recently, it has become possible to exactly simulate quantum dynamics using advanced methods based on tensor networks [2]. Using these and other methods we have shown how the interactions between a qubit and its environment, which are necessary for reset, also limit its performance, and how this can be overcome [3]. So far, however, our work has been on an idealized model of a qubit interacting with a reservoir. In this project you will build a realistic model of the superconducting qubit system, comprising a transmon qubit coupled to a waveguide resonator [1], and explore theoretically both the limitations on reset and how they can be overcome.

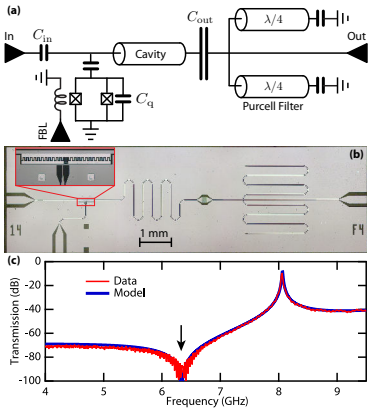



Figure 1: Reproduced from Ref. [1]. Design and realization (a,b), and diagnostic transmission data (c) for a Purcell filter system used to implement transmon reset.

## References

[1] M. D. Reed, B. R. Johnson, A. A. Houck, L. DiCarlo, J. M. Chow, D. I. Schuster, L. Frunzio, and R. J. Schoelkopf, "Fast reset and suppressing spontaneous emission of a superconducting qubit", Applied Physics Letters **96**, 203110 (2010).

[2] G. E. Fux, P. Fowler-Wright, J. Beckles, E. P. Butler, P. R. Eastham, D. Gribben, J. Keeling, D. Kilda, P. Kirton, E. D. C. Lawrence, B. W. Lovett, E. O'Neill, A. Strathearn, and R. De Wit, "OQuPy: A Python package to efficiently simulate non-Markovian open quantum systems with process tensors", The Journal of Chemical Physics **161**, 124108 (2024).

[3] C. Ortega-Taberner, E. O'Neill, and P. Eastham, *Quantum control of the environment in open quantum systems enables rapid qubit reset*, arXiv.org, (Mar. 10, 2026) https://arxiv.org/abs/2603.09913v1 (visited on 05/26/2026).

# ML models for materials designed by AutoResearch

Supervised by Prof. Stefano Sanvito

## Background

AutoResearch is a new agentic AI tool for scientific workflow automation [1]. In practice, it uses an iterative reasoning process powered by large language models to design and perform assigned tasks. This allows to drastically speed up the creation and execution of complex workflow. The idea of the project is to use such a new tool to create machine-learning (ML) models for materials discovery, for example for the prediction of the ferromagnetic critical temperature of magnets or the bandgap of insulators and semiconductors [2].

## Objectives

The project seeks to use AutoResearch for the construction of ML models for the prediction of some specific materials quantities (e.g. the critical temperature of superconductors, the bandgap of insulators, etc.). In particular, we will consider two tasks: 1) the optimization of the materials descriptors (the characteristic properties that define a material); 2) the structure and parameters of the ML model.

## Tasks

The student will first familiarise with the AutoResearch framework. Then, they will set up the problem and initiate the iterative steps. In a first phase, the datasets needed for the models will be provided. If proved successful, we will explore the possibility to use AutoResearch also for the creation of the initial dataset. In this case, AutoResearch will be used to mine the literature and extract the relevant information.

# References

[1] Guiyao Tie, Jiawen Shi, Dingjie Song, Yixiao Huang, Ziji Sheng, Xueyang Zhou, Daizong Liu, Pan Zhou, Yongchao Chen, Ran Xu, Lifang He, Qingsong Wen, Manling Li, Cong Lu, Shuai Li, Pengtao Xie, Yixuan Yuan, Rui Meng, Lei Xing, Lichao Sun, Caiming Xiong, Philip S. Yu and Jianfeng Gao, *AutoResearch AI: Towards AI-Powered Research Automation for Scientific Discovery*, arXiv:2605.23204 (2026).

[2] Matteo Cobelli and Stefano Sanvito, *Agentic Design of Compositional Descriptors via Autoresearch for Materials Science Applications*, arXiv:2605.14671 (2026).

# Creating an atomic DFT code with AI

Supervised by Prof. Stefano Sanvito

## Background

Density functional theory (DFT) is an in-principle exact theory to solve any quantum many-body electronic problem. The main idea is rooted in the Hohenberg-Kohn theorems [1], which establish that 1) the total energy of a many-body electronic system is a universal functional of the single-particle density, $n(\mathbf{r})$, and that 2) the functional is minimised at the ground-state density, returning the ground-state energy. Being universal, DFT can then solve any quantum mechanical problem and can describe the electronic structure of atoms, molecules and solids. Unfortunately, the exact many-body functional is not known, but accurate approximations exist, so that DFT is also a practical theory.

## Objectives

In this project we will construct a DFT code to compute the electronic structure of atoms. This was used to be a daunting task only a few months ago, but today AI enables the rapid writing of efficient computer code. The project will involve the construction of a small DFT code including an appropriate self-consistent numerical solver. We will consider the most simple approximation to DFT, namely the local density approximation (LDA) and the generalised gradient approximation (GGA).

## Tasks

The first task is to familiarise with the main concepts behind DFT and how a numerical implementation can be constructed. Then, we will start building a numerical solver for the nuclear potential, with the wave-function written as a linear combinations of spherical harmonics and numerical radial grid. The final goal is that of computing the spectrum (eigenvalues) and the total energy of light atoms (H, He, Li ...).

# References

[1] P. Hohenberg and W. Kohn, *Inhomogeneous Electron Gas*, Phys. Rev. **136**, B864 (1964).

[2] W. Kohn and L.J. Sham, *Self-Consistent Equations Including Exchange and Correlation Effects*, Phys. Rev. **140**, A1133 (1965).

# Phase stability predictions with foundational force fields

Supervised by Prof. Stefano Sanvito

## Background

The phase stability of a given compound can be assessed (at least at zero temperature) by comparing its total energy with that of the potential competitive compounds (those a material it can decompose into). This is usually calculated by using some electronic structure theory of some sort, most typically density functional theory (DFT), often a computationally intensive task. Recently, efficient foundational (which apply to all materials) force fields have been developed [1]. These offer high accuracy in determining the total energy of a material and little computational overheads. However, whether these are accurate enough to determine phase diagram remains an open question.

## Objectives

The project seeks to use foundational force fields for the calculation of convex hull diagrams for a range of binary and possibly ternary phases [2]. If time will allow, we will also investigate the possibility of exploring new compounds in the search for novel phases never grown in the lab before.

## Tasks

The student will first familiarise with the concept of convex hull diagram and with machine-learning force fields. Then, we will consider some of the phase diagrams computed in the AFLOWLIB.org database [3], for both intermetallic compounds and systems containing main-group elements, and attempt at reproducing them with the force field. We will consider both relaxed and unrelaxed structures and evaluate the fidelity of the force field against DFT data. Finally, if the time allows, we will develop a generative strategy and explore the stability of novel phases never attempted before.

# References

[1] Ilyes Batatia, et al., *A foundation model for atomistic materials chemistry*, J. Chem. Phys. **163**, 184110 (2025).

[2] Hugo Rossignol, Michail Minotakis, Matteo Cobelli and Stefano Sanvito, *Machine-Learning-Assisted Construction of Ternary Convex Hull Diagrams*, J. Chem. Inf. Model. **64**, 1828 (2024).

[3] Stefano Curtarolo, Wahyu Setyawan, Shidong Wang, Junkai Xue, Kesong Yang, Richard H. Taylor, Lance J. Nelson, Gus L.W. Hart, Stefano Sanvito, Marco Buongiorno-Nardelli, Natalio Mingo and Ohad Levy, *AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations*, Comp. Mater. Sci. **58**, 227 (2012).

**Real-Time Scientific Visualization – Volume Rendering of Scalar and Vector Fields – Towards an Ultra-Light and User- and Hardware-Friendly Display Engine - Stamenov (Computation)**

Modern computer hardware allows for unprecedented access to parallel graphics and neural networks-accelerated rendering, including for scientific visualization purposes. The use of mixed CPU-GPU strategies for volume rendering of scalar and vector fields is beginning to take hold, but the availability of customizable, real-time control and display engines is very limited. While the contemporary gaming industry has gone a step further, by utilizing specialized NPU accelerators even in inexpensive consumer grade hardware, the scientific visualization community is still playing catch...

Here we propose to build upon existing work by the PI on a real-time volume rendering engine, which allows for a real-time control (navigation and colorization) of large volume datasets (both scalar and vector ones), and provide user-friendly interface and a number of input filters – for the direct input of scientific datasets (from the results of DFT calculations, through medical imaging data, to experimental magnetic field mappings and beyond), and gradient tensor visualization enhancers, to name three specific areas.

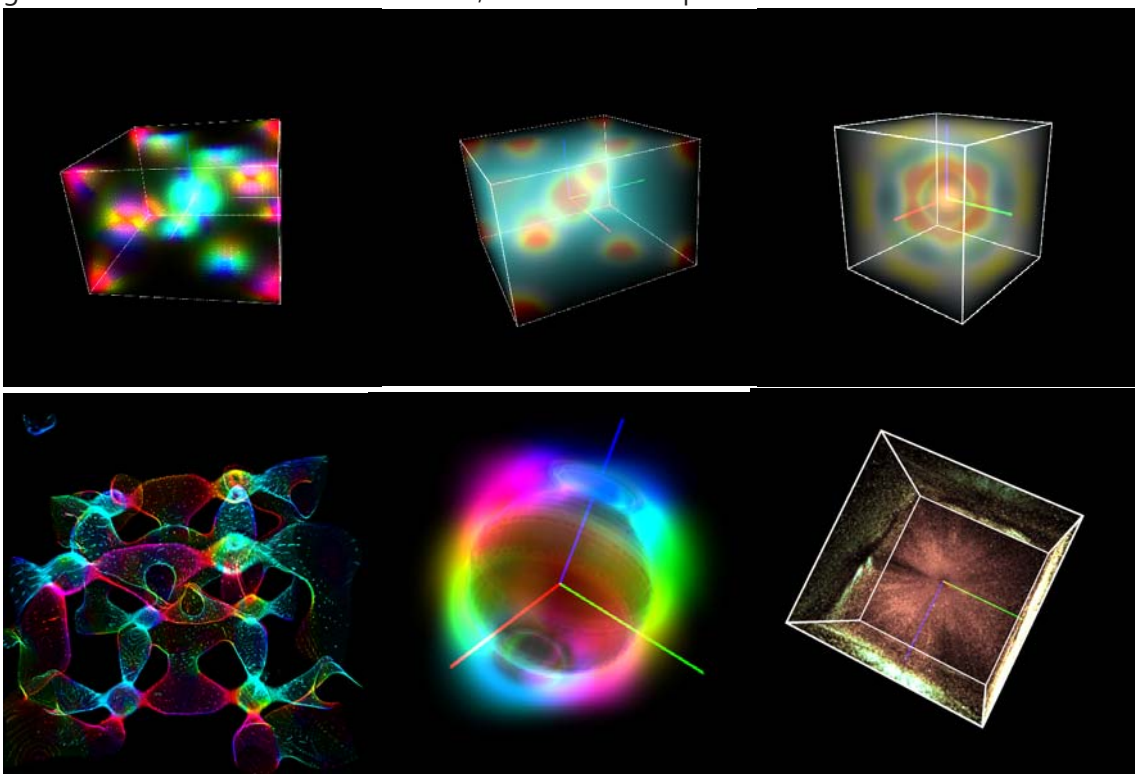


Fig. 1. Snapshots of the real-time video rendering stream of the current version of the Trinity Ray Caster. Left-to-right, top-to-bottom: The real-space spin distribution in the altermagnetic-candidate material ruthenia; the excess charge distribution in the same; the real-space exchange field in bcc iron; the spin-polarised hole Fermi surface of ruthenia; the non-homogenous part of the vector magnetic induction of a metrological coil design; and a volume rendering of the stars in the Milky Way galaxy and its near vicinity (the large and small Magellanic clouds can be seen to left). Depending on the exact hardware, dataset size and rendering resolution settings, the engine can push 10 – 150 FPS.