SURE Projects 2025

L'indirizzo email della persona che ha risposto (**t.e.muller-bravo@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

t.e.muller-bravo@tcd.ie

Project Title *

Studying Type Ia Supernovae Through Their Colour Evolution

Supervisor(s) *

Dr. Tomás Müller Bravo, Prof. Kate Maguire

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Type Ia supernovae (SNe Ia) are thermonuclear explosions of white dwarfs in binary systems, serving as crucial tools for measuring cosmic distances and probing the expansion rate of the universe. Their luminosity is influenced by both intrinsic properties and external factors such as dust extinction from their host galaxies, thus affecting the estimated distances. In addition, the exact nature of their explosion is still unknown. This study will examine the colour evolution of thousands of SNe Ia recently observed by the Zwicky Transient Facility (ZTF; [1]) to infer constraints on progenitor systems and dust extinction. The student will use multi-band (gri) light curves of well-sampled SNe Ia to calculate the colour evolution (g-r, r-i) as a function of phase, focusing primarily on late-phase evolution to study the Lira Law [1], and also on early-phase behaviour such as the colour bimodality [3]. The student will code in Python to analyse the data and use advanced statistical methods to investigate correlations. Machine-learning techniques can be applied depending on the interest of the student. The results will provide new constraints on dust extinction and offer insights into the environments and progenitor systems of SNe Ia, advancing our understanding of their physical and astrophysical properties.

Reference [1]: Rigault, Smith, Goobar et al. arXiv, arXiv:2409.04346, 2024
https://ui.adsabs.harvard.edu/abs/2024arXiv240904346R/abstract
Reference [2]: Phillips, M. M., Lira, P., Suntzeff, N. B., et al. 1999, AJ, 118, 1766
https://ui.adsabs.harvard.edu/abs/1999AJ....118.1766P/abstract
Reference [3]: Stritzinger, M. D., Shappee, B. J., Piro, A. L., et al. 2018,
ApJL, 864, L35 https://ui.adsabs.harvard.edu/abs/2018ApJ...864L..35S/abstract

Students tasks *

collect the supernova light curves, calculate their colour evolution and apply statistical method using Python

Essential prerequisites

interest in supernovae and coding in python

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**stefan.hutzler@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

stefan.hutzler@tcd.ie

Project Title *

Experiments with crystalline foams

Supervisor(s) *

Stefan Hutzler

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

Equal volume soap bubbles order spontaneously in crystalline arrangements when collected in cylinders of diameter similar or slightly larger than the bubble diameter. Rearrangements into alternative structures can be achieved by adding liquid at controlled flow rates onto such vertical columnar crystals. This project will study such transitions, and also the propagation of grain boundaries, similar to those known in metallography. It will also be explored how a heated surfactant solution can be used for the creation of equal volume bubbles.

Students tasks *

Setting up various types of columnar crystals made of bubbles. Identification and imaging of the structures. Production of high quality videos of structural transitions. Development of a set-up for making monodisperse foam using a heated surfactant solution.

Essential prerequisites

Love of experimental work and playing around with simple equipment. Making videos.

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**crossg@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

crossg@tcd.ie

Project Title *

Assembly of Patterned Surface Coatings For Superlubricious Applications

Supervisor(s) *

Graham Cross

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

Mechanical components suffer severe energy losses and degradation from friction between moving parts, costing billions in dollars of losses across a range of industries every year. This is reduced significantly by the introduction of lubricants on the interacting surfaces. Typical liquid lubricants like motor oil reduce friction between parts moving at high speeds or at low contact pressures by preventing rough surfaces from scraping against each other. However, contact at high pressures and/or slow speeds experience high friction even with traditional liquid lubricants, a contact regime known as boundary lubrication. One of the ways to reduce friction in this regime is by careful patterning of the contact surfaces to reduce contact area between the contact bodies. Performing this patterning at the micron scale allows for reduced friction between surfaces that appear otherwise flat on macro scale components. Several patterning geometries to reduce friction exist, including arrays of spherical bumps which reduce surface contact to that between the sphere tips at twisted contact angles.
This project will explore the self-assembly of microspheres on flat surfaces, whereby dispersions of monodisperse microspheres are deposited onto a liquid interface and allowed to assemble into a close-packed structure, before being deposited on a flat substrate. This assembly process is limited by a number of factors including the size of the spheres, and experiences point defects and grain boundaries between aligned pattern regions. The aim of this project is to explore the effect of microsphere size and deposition method on the resulting assembled close-packed structure and the presence of defects. Experimental data will be compared with known theory on assembled structure via surface energy considerations. Results obtained will provide insight on the development of mass producible surface structures for superlubricious surfaces.

Students tasks *

- Cleaning and preparation of substrates for microsphere deposition
- Deposition of microspheres on to a variety of substrates
- Optimising deposition methods for various microsphere sizes
- Characterisation of sphere assemblies via optical and electron microscopy
- Coating of sphere assemblies with superlubric furnace grown thin films
- Characterisation of growth process of furnace grown coatings

Essential prerequisites

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**n.gibson@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

n.gibson@tcd.ie

Project Title *

Atmospheres of alien worlds: exploring new tools for tranmission spectroscopy of exoplanets

Supervisor(s) *

Neale Gibson

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Exoplanets are simply planets that orbit stars other than our Sun, and thousands have been discovered over the last few decades. A key frontier for astronomers is to try and characterise these planets in detail through spectroscopy of their atmospheres, which allows us to measure atmospheric temperatures and compositions, which in turn allows us to figure out the main physical and chemical processes that shape these worlds. The long term goal is to apply these methods to potentially habitable worlds, and even to search for 'biomarkers' - signs of extraterrestrial life.

Students tasks *

This project will use data from the James Webb Space Telescope (JWST) or a large ground-based facility like ESO’s Very Large Telescope to extract a spectrum of an exoplanet, allowing us to probe the chemistry and physical properties of the atmosphere. This project will focus on data analysis and statistics. The student will spend most of their time writing python code to analyse light curves and/or time-series spectra to extract an exoplanet's spectrum. Depending on the interests of the student, there may also be opportunities to study atmospheric physics and apply modelling techniques to understand the atmosphere.

Essential prerequisites

Knowledge of computer programming is essential. Experience of python would be valuable.

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**hozhang@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

hozhang@tcd.ie

Project Title *

Plasma engineering of two-dimensional MoS2 edges for next-generation electronics

Supervisor(s) *

Hongzhou Zhang

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

This project explores an innovative approach to tailoring the edge properties of two-dimensional (2D) MoS_2 flakes through plasma treatment. As a key member of the Transition Metal Dichalcogenide (TMD) family, MoS_2 holds immense promise for next-generation electronic and optoelectronic devices, including Field-Effect Transistors (FETs), photodetectors, and memristors. [1,2,3] However, as these devices shrink in size, their performance increasingly depends on edge structures, which play a crucial role in electronic behaviour and power consumption. [4, 5]
By precisely tuning the edges of 2D MoS_2, we can unlock enhanced electronic, nonlinear optical, and photoluminescence properties, paving the way for more efficient nanoscale devices. Despite its transformative potential, large-scale, reliable edge engineering of MoS_2 remains largely unexplored. Plasma treatment presents a powerful solution, offering fine control over the morphology of 2D flakes and enabling targeted modulation of their electrical, chemical, and optical characteristics.
In this project, an oxygen plasma tool will be employed to modify large-area Chemical Vapor Deposition (CVD)-grown 2D MoS_2 flakes, with the goal of refining their microstructures for optimized performance. The structural and optical transformations induced by plasma treatment will be analysed using state-of-the-art techniques, including Atomic Force Microscopy (AFM), Raman spectroscopy, and photoluminescence (PL) spectroscopy.
Participants will gain hands-on experience in cutting-edge nanomaterial synthesis and characterization, including CVD growth of 2D MoS_2, optical and structural analysis techniques, and plasma-based modification methods. This study will provide critical insights into plasma-induced nanoscale engineering, contributing to the future design of high-performance 2D electronic and optoelectronic devices.
Reference:
[1] J. Jadwiszczak, et al. “Oxide-mediated recovery of field-effect mobility in plasma-treated mos2,” Science advances, vol. 4, no. 3, p. eaao5031, 2018.
[2] J. Jadwiszczak, et al. “Photoresponsivity enhancement in monolayer mos2 by rapid o2: Ar plasma treatment,” Applied Physics Letters, vol. 114, no. 9, 2019.
[3] V. K. Sangwan et al. “Multi-terminal memtransistors from polycrystalline monolayer molybdenum disulfide,” Nature, vol. 554, no. 7693, pp. 500–504, 2018.
[4] W. Cao, et al. “The future transistors,” Nature, vol. 620, no. 7974, pp. 501–515, 2023.
[5] F. Zhang, et al. “Exploration of channel width scaling and edge states in transition metal dichalcogenides,” Nano Research, vol. 11, pp. 1768–1774, 2018.

Students tasks *

Reading literatures; Participate in research discussions; Receive hands-on trainings on materials growth/synthesis; conduct experiments; analyse/communicate results;

Essential prerequisites

Basic lab skills; basic programming skill; analytical/critical thinking; teamwork;

Google Moduli

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**hozhang@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

hozhang@tcd.ie

Project Title *

Precise p-type doping of two-dimensional MoS2 via niobium source tuning in Chemical Vapor Deposition

Supervisor(s) *

Hongzhou Zhang

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

This project aims to achieve precise p-type doping in MoS_2 and optimize its structural properties with a focus on controllability, uniformity, and wafer-scale growth. MoS_2 is an intrinsic n-type semiconductor, while p-type doping is particularly essential for the formation of p-n junctions, which are fundamental in devices such as LEDs, lasers, photodiodes, and high-performance field-effect transistors (FETs), where efficient charge carrier injection, extraction, and reduced contact resistance with metal electrodes are required. Although substitutional Nb doping for p-type conduction in MoS_2 has been explored via CVD, achieving uniformity and precise doping control remains challenging. This project utilizes a polymer-assisted spin-coating technique with a CVD system to introduce niobium precursors separately, enabling better doping regulation. Optimizing temperature, gas flow, and precursor delivery is crucial for obtaining large-area, continuous MoS_2 flakes with well-defined doping densities. This study aims to precisely control doping levels between 0.5% and 20% in monolayer MoS_2 and evaluate their impact on flake uniformity, size, and electronic performance.

To characterize the doped material, optical microscopy and scanning electron microscopy (SEM) will be used to examine the morphology and grain boundaries of the flakes. Atomic force microscopy (AFM) will provide insight into thickness and surface topology, while Raman spectroscopy and X-ray diffraction (XRD) will be employed to analyze crystal orientation, phase purity, and strain effects. High-resolution transmission electron microscopy (HRTEM) will reveal atomic-scale microstructures, while X-ray photoelectron spectroscopy (XPS) and energy-dispersive X-ray spectroscopy (EDX) will confirm and quantify doping concentrations. For device fabrication, photolithography techniques will be applied, and electrical measurements, using a low-temperature four-probe station and a semiconductor analyser, will be conducted to assess the memristive and optoelectronic properties of the doped material.

This project provides extensive hands-on training in CVD-based doping techniques, with a focus on parameter optimization to achieve precise doping control. Additionally, participants will develop expertise in advanced material characterization methods, including Raman spectroscopy, photoluminescence, AFM, SEM, and EDX, along with sample preparation techniques. Training will also cover essential device fabrication methods such as 2D film transfer, spin coating, optical lithography using a mask aligner, and metal deposition through electron beam evaporation. By systematically exploring controlled doping strategies in 2D materials, this research will contribute to the advancement of next-generation electronic and optoelectronic devices, offering insights into the role of defect engineering in tailoring material properties.

References:

1. Dolui, K. et.al. (2013). Possible doping strategies for MoS 2 monolayers: An ab initio study. Physical Review B—Condensed Matter and Materials Physics, 88(7), 075420.
2. Li, M., et.al. 2020). P-type doping in large-area monolayer MoS2 by chemical vapor deposition. ACS applied materials & interfaces, 12(5), 6276-6282.
3. Gao, H., et.al. (2020). Tuning electrical conductance of MoS2 monolayers through substitutional doping. Nano Letters, 20(6), 4095-4101.
4. Loh, L., et.al. (2021). Substitutional doping in 2D transition metal dichalcogenides. Nano Research, 14, 1668-1681.
5. Pham, V. P., et.al. (2016). Recent advances in doping of molybdenum disulfide: industrial applications and future prospects. Advanced Materials, 28(41), 9024-9059.

Students tasks *

Literature review; trainings on CVD and other characterisation techniques; conduct experiments; analyse/report results

Essential prerequisites

basic lab skills; analytical/critical thinking; teamwork; time management; basic coding skills

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**MULLANIN@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

MULLANIN@tcd.ie

Project Title *

Recognition and Optimization of Monolayer MoS2 Growth on Photoresist Coated Substrates

Supervisor(s) *

Navaj Bapuso Mullani

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

Recognition and Optimization of Monolayer MoS2 Growth on Photoresist Coated Substrates
Abstract: This project aims to improve monolayer molybdenum disulphide (MoS2) growth efficiency within a photoresist (PR)-coated substrate area by developing and modifying recognition methods for CVD-grown monolayer regions using characterization techniques such as AFM and Python-based data analysis. Achieving uniform and efficient monolayer MoS2 growth is critical for advancing 2D material applications in nano and optoelectronics. Our current studies show the use of S1813 diluted polymer as a promoter for nucleation plays a pivotal role in controlling growth. However, accurately recognizing, quantifying monolayer areas among the PR-coated substrate remains an intricacy, limiting the optimization of growth conditions and material yield. While nucleation promoters aid in MoS2 growth, the precise identification of monolayer regions and their relation to nucleation centers has not been amply explored. Most of the literature has only recognized or grown monolayer regions. Developing a viable method to recognize and quantify these regions efficiently is crucial, as well as understanding how this recognition relates to optimizing the growth process. The project will use atmospheric pressure CVD (APCVD) to grow monolayer MoS2 on PR-coated substrates prepared with S1813 (with multiple dilutions) polymer. Post-growth, AFM will be employed for surface characterization, and Python programming will be used to develop a recognition algorithm for identifying monolayer regions. The identified areas will be correlated with nucleation centers to refine growth efficiency and uniformity. This project will provide students with substantial knowledge and training in CVD growth of 2D materials, optical and surface characterizations mainly, Raman/PL/AFM, and Python-based data analysis. It will contribute to developing new methods for improving monolayer growth efficiency and create a systematic approach for identifying monolayer regions within PR-coated areas.

References:
1) Understanding epitaxial growth of two-dimensional materials and their homostructures | Nature Nanotechnology
2) Conformal Growth of Nano-Patterned Monolayer MoS2 with Periodic Strain via Patterned Substrate Engineering for High-performance Photodetectors - Jian - 2025 - Laser & Photonics Reviews - Wiley Online Library
3) Wafer-scale and deterministic patterned growth of monolayer MoS2 via vapor–liquid–solid method - Nanoscale (RSC Publishing)
4) Monolayer MoS2 Transferred on Arbitrary Substrates for Potential Use in Flexible Electronics | ACS Applied Nano Materials

Students tasks *

Take trainings; conduct experiment; analyze/report data; attend meetings/discussions

Essential prerequisites

basic lab skills; analytical/critical thinking; teamwork; communication skills

Google Moduli

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**lmatra@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

lmatra@tcd.ie

Project Title *

First Infrared Measurement of the 13CO/12CO ratio in Exocometary Gas with VLT/CRIRES+ Spectroscopic Observations

Supervisor(s) *

Luca Matrà and Kevin Smith

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

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 (Matrà et al. 2025). While these were previously thought to be gas-free, observations now have the sensitivity to detect gas, particularly carbon monoxide (CO), released from exocometary ices within the belt (see Interstellar Objects and Exocomets chapter in Comets III book).
An exciting, yet unpublished result at mm wavelengths with the Atacama Large Millimeter/submillimeter Array (ALMA) has been that the ratio of 12CO/13CO, the main and rarer isotopologues of the CO molecule, is very low (~2). This is surprisingly low compared to the typical values measured in the interstellar medium (~77) and in the Solar System (~90). As isotopologue ratios such as 12CO/13CO are typically used to trace back our chemical origins, it is important to confirm and understand the cause of this surprisingly low value in exocometary gas - especially since exocomets may deliver their ices to forming terrestrial planets in this era.
The first step towards this, and the goal of this project is to confirm the 12CO/13CO measurements from ALMA, using independent observations at infrared (IR) wavelengths with the new CRIRES+ high resolution spectrograph on the Very Large Telescope (VLT). In particular, the project will focus on fitting the 13CO rovibrational absorption lines from the exocometary gas observed against the background starlight, in the two edge-on belts around ~15 Myr-old HD110058 (Hales et al. 2022) and HD131488 (Pawellek et al. 2024). Combining derived column densities with the 12CO column density already obtained (Smith et al. in. prep., Brennan et al. 2024) will enable the first IR measurement of the 12CO/13CO ratio in exocometary belts, and confirm/refute the measurements in emission obtained by ALMA.

Students tasks *

Analysing new CRIRES+ data (spectra) from the VLT
[Correcting for telluric absorption lines with Molecfit package]
Fitting model absorption lines to multiple detected 13CO transitions
Measure 12/13CO ratio and confirm/refute ALMA result

Essential prerequisites

Python (using packages/functions, plotting, array manipulation), ideally having taken Astrophysical Spectroscopy course PYU33A17

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**Stephen.Dooley@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

Stephen.Dooley@tcd.ie

Project Title *

Automated Exploration and Mechanistic Analysis of the Xylopyranose Decomposition Reaction Network

Supervisor(s) *

Stephen Dooley, Bernardo Ballotta

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Understanding the chemical reactivity linked to biomass pyrolysis is still a topic of debate in the scientific community. Although numerous experimental investigations have been conducted in recent decades to study these chemical systems, the reaction mechanisms that characterize their pyrolisis are still unclear. Thanks to the recent development of computational modeling techniques it is now possible to study and analyze complex systems such as biomass in detail. In particular, the use of programs for the automated search of reaction mechanisms appears to be a promising methodology to obtain an exhaustive characterization of the possible decomposition channels of the units that make up biomass, significantly reducing the possibility of neglecting fundamental reaction channels. In this work, the β-D-Xylopyranose decomposition reaction network is studied using the program for automated reaction mechanism discovery AutoMeKin, which combines reactive molecular dynamics simulations, post-processing of data obtained for the selection of the transition states participating in the reaction mechanism and DFT optimization of stationary points. The application of these methodologies to other systems of interest for biomass pyrolysis could contribute to a greater understanding and prediction of their chemical reactivity.

Students tasks *

Selection of relevant chemical pathways in pyrolysis, structure optimization, vibrational analysis, electronic energy refinement of reactive potential energy surfaces for xylopyranose decomposition.

Essential prerequisites

Familiar with linux, bash and python.

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**johanna.vos@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

johanna.vos@tcd.ie

Project Title *

Calculating Gas Opacities for the JWST Era

Supervisor(s) *

Johanna Vos, Evert Nasedkin (Postdoc)

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Gas opacities are critical datasets for interpreting and fitting observations of exoplanets and brown dwarfs, allowing us to peer into their atmospheres to search for molecules such as water, carbon monoxide and methane. High resolution line lists provide the most accurate method for identifying features in observed spectra, but are too large to be used in fitting lower resolution observations. With JWST's broad wavelength coverage and high spectral resolution, new opacity tables are necessary in order to exploit these new observations. This project would have the student computing correlated-k opacity tables to be included in the widely-used petitRADTRANS software. These would be the first such opacity tables designed for use specifically with JWST observations, and will enable critical new analysis of sub-stellar atmospheres.

Students tasks *

The student will use python to create opacity tables for all species of interest in exoplanet and brown dwarf atmospheres. These will be incorporated into one of the main atmospheric analysis codes used by exoplanet scientists today, and used to search for molecules and other species in the atmosphere of worlds beyond our solar system.

Essential prerequisites

python

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**Stephen.Dooley@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

Stephen.Dooley@tcd.ie

Project Title *

Experimentally Prescreening Sustainable Aviation Fuels

Supervisor(s) *

Stephen Dooley

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

Sustainable aviation fuel (SAF) is crucial to the decarbonisation of the aviation industry as it represents the only viable pathway. By 2050, the European Union require that all aviation activities have net zero emissions, currently there is not enough feedstock, or production in the topic for this happen. As part of SAF development, prescreening is performed to give early certification on a candidates SAF's likelihood of passing strict safety and testing standards. Prof. Stephen Dooley's Low Carbon Technologies' research group are proactively contributing to this space by developing research methods through work at the SAF LAB, a cutting-edge laboratory containing 14+ analytical devices.

As part of the SURE project, you will be trained on these devices to calibrate and standardise measurements to be used as a basis against for the candidate SAF samples. This measurement campaign is vital to progress of SAF development as it will allow fuel producers to see if their fuel sample complies with conventional fuels, which is currently a large finical hurdle due to quantities of fuel needed for full certification without early assessment.

Students tasks *

- Trained on experimental equipment
- Make measurements on standard components
- Calibrate the device for use in prescreening
- Standardize the device with mixtures

Essential prerequisites

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**easthamp@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

easthamp@tcd.ie

Project Title *

Quantum heat engines using light

Supervisor(s) *

Paul Eastham

Type of project *

- (●) Theoretical
- ( ) Computational
- ( ) Experimental

Project description *

A quantum heat engine is a device which, like its classical counterpart, converts heat to work. They provide a key theoretical paradigm for understanding how quantum-mechanical effects, such as superposition and entanglement, can impact on the operation and performance of machines. However, most experiments on quantum heat engines involve challenging work on systems such as single atoms at low temperatures. In this project you will investigate theoretically how a quantum heat engine could be constructed by trapping photons in optical cavities and allowing them to cool as they interact with a dye at room temperature. You will extend and study a model of these devices, which describes the kinetics of the photons cooling within the device, and explore the extent to which quantum effects can improve their performance.

Students tasks *

The first tasks of this project involve constructing kinetic equations, for the photon occupations in the cavity, based on available literature and our previous work, and identifying effective means to analyse them. This may include anaytical approaches and numerical simulations, in Mathemtica or Python. You will use these to evaluate the performance across various parameters, with the goal of identifying how the reversible limit can be achieved, and whether it can be done so at finite power. Beyond this, you will construct equations-of-motion describing the quantum fluctuations, from an open quantum-systems approach, and solve them in a similar way. This will allow us to establish the role of quantum effects, and predict how they could be probed in experiments.

Essential prerequisites

Interest in quantum mechanics and theory, as well as making connections to experiments. Confident user of mathematical and computational tools in physics.

SURE Projects 2025

L'indirizzo email della persona che ha risposto (**lunghia@tcd.ie**) è stato registrato quando hai inviato questo modulo.

Email *

lunghia@tcd.ie

Project Title *

Simulating quantum decoherence in molecular qubits

Supervisor(s) *

Alessandro Lunghi

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Quantum systems can retain their state for a finite amount of time, namely their coherence time. The stronger the interaction between the quantum systems and its enviornment the shorted the coherence time is, thus limiting the possibility to use condensed-matter systems for quantum technologies. Understanding the details of decoherence is essential to mitigate it and possibly realize materials that can exhibit robust quantum features. The goal of this project is to use cluster correlation expansion methods to compute the decoherence mechanism and coherent time of molecular spin in solid-state enviornment.

Students tasks *

The project is mainly computational in nature and the student assigned to it will be in charge of running numerical simulations witht the Python library PyCCE. The student will then use quantum mechanics to interpret the results and explain the nature of decoherence for molecular spin.

Essential prerequisites

Excellent skills with Python; good understanding of quantum mechanics