Senior Sophister Projects 2020/21

School of Physics,
Trinity College Dublin
Please fill out the form at the following location depending on whether you are a Physics, Physics and Astrophysics or Nanoscience student:

Physics Choice Form
Physics and Astrophysics Choice Form
Nanoscience Choice Form

Students in Physics should **only** choose from projects numbered **1 to 53**
Students in Physics and Astrophysics may choose from projects numbered **1 to 71**
Students in Nanoscience may choose from projects numbered **1 to 53** in this document and any from the SS Projects for Nanoscience booklet.

Nanoscience students: Please consider choosing from both Physics and Chemistry lists to even the distribution of projects. Use the alphanumeric code, e.g. BB1, when choosing a Chemistry project on survey monkey and the project number when choosing a Physics project.

For further details about projects contact the named project supervisor.
For general information about projects, contact [Prof. Patterson](mailto:professor.patterson@university.com)
For general course information, contact the course director:
Prof. McGuinness (Physics)
Prof. Groh (Physics and Astrophysics)
Prof. Dunne (Nanoscience)

PLEASE COMPLETE THE PROJECT CHOICE FORMS BY FRIDAY 21st August 2020.
You MUST select **six projects** in order of your preference. There is also a section of the project choice forms which asks whether you have your own laptop and broadband to allow you to work remotely.
1 List of Physics Projects

1. Bandgap Renormalization in Nanolayered PtSe₂
2. Rate equation simulations of ultrafast population dynamics in large organic molecules and nanostructures
3. From Purcell (weak) to Rabi (strong) light-matter interaction with coupled 2D materials and nanoantenna
4. Tunable metasurfaces and reflect-arrays
5. XPS analysis of oxide interfaces with MRG
6. ARPES analysis of Fermi level band spectra in various sputtered/PLD films
7. Ultrafast sublattice resolved magnetisation dynamics in ferrimagnets
8. Magnetic Water Treatment
9. Nanobubble water
10. In-situ imaging of magnetic domains generated by single femtosecond light pulse
11. Printed supercapacitors from graphene and boron nitride nanosheets
12. Nanomechanical characterization of self-assembly in novel 2D materials
13. Optically detected magnetic resonance of diamond nitrogen-vacancy centers
14. Study of wavelength tuning in 1.3 micron laser array
15. Athermalisation of semiconductor lasers operating at 1.3 and 1.5 microns
17. Data Mining and Principal Component Analyses of Rapid Compression Machine Ignition Physics
18. Spin transport in organic materials
19. Decoding the disorder signatures in conductance calculations: A quantum inverse problem
20. Steady-state thermodynamics of composite collision models
21. Many-body localized dynamics
22. Quantum dynamics of an impurity in a cold fermionic gas
23. Quantitative diagnostics of corona virus proteins or immune responses to the virus in biological liquids
24. Single Photons in the Vicinity of an Optical Black Hole
25. Winner-loser models
26. Buckling of a linear chain of hard and soft spheres (ball-bearings, soap bubbles) in a confining potential
27. Doubling Electron Microscope Video-rates Using Frame Interlacing
28. Using video-game GPUs to better predict focus-blur in the Transmission Electron Microscope
29. Optimized antireflection coatings for Rooftop Solar PV
31. Modelling of novel heat exchanger for Solar Thermal Applications
32. Simulation of electronic structure, scanning tunnelling microscopy and spectroscopy of new porphyrin-derived on-surface synthesized porphyrin nanoribbons
33. X-ray magnetic circular dichroism of few atom-wide capped cobalt nanowire arrays
34. Theoretical simulation of x-ray absorption and resonant inelastic x-ray scattering in transition metal oxides
35. The packing structure of disordered platelet suspensions
36. Splashing droplets
37. Testing a new fast method for predicting the gap of metal oxides
38 Simulation of Stokes shifts in light emission by organic materials
39 Many-body theory of exciplexes for OLED devices
40 Molecular dynamics of materials with light emitter applications
41 Electronic states in defected fractal lattices
42 Optical Investigations of a-Zinc Tin Oxide films deposited via spray pyrolysis
43 Quasi-classical spin dynamics in compensated ferrimagnetic systems approached to understanding pinning and nucleation of domain walls and skyrmions
44 High-Power Narrow (K and Ka)-Band Waveguide-based Ferromagnetic Resonance in Thin Magnetic Films and Microstructures: Simultaneous inductive and SQUID-based Detection
45 Sub-picosecond pulsed induced demagnetisation of magnetic materials: resolving the role of the exchange interaction
46 Anisotropy of the Conductivity and Hall Effect in Zero-Moment Half-Metallic Systems
47 Machine learning density functional theory at finite temperature
48 Machine-learning force fields for the phase diagram of oxides
49 Machine learning density functional theory for electron-phonon models
50 Can machine learning understand molecules?
51 Understanding the origins of luminescence tuning in ZnO nanostructures via ion irradiation

List of Astrophysics Projects
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55 City light output in the time of COVID-19
56 High Speed Monitoring of Solar Radio Bursts
57 Atmospheres of alien worlds: exploring transmission spectra of exoplanets using machine-learning techniques
58 Atmospheres of alien worlds: searching for new atmospheric species via high-resolution transmission spectra
59 Atmospheres of alien worlds: exploring new tools for high-resolution transmission spectra of exoplanet atmospheres
60 Stars that directly collapse to black holes
61 The properties of the first stars in the Universe
62 Effects of stellar populations in the nearby Universe
63 How does explosive magnetic reconnection in Saturns magnetosphere drive intense radio emissions?
64 Radio emission from nebulae around massive stars
65 Spectroscopic modelling of thermonuclear supernovae
66 Unveiling the explosion geometries of massive-star supernovae
67 Type Ia supernovae: Cosmology and their explosion properties
68 Statistics of Solar Eruptions
69 Leaky atmospheres in exoplanets: the strength of H-alpha transits
70 The role of the tachocline in stellar magnetic field generation
71 Modelling the propagation of cosmic rays in protoplanetary disks observed with ALMA
Inorganic nanosheet materials are emerging as a new platform for exploring semiconductor physics in two dimensions. Reduced screening in two dimensions results in distinctly enhanced electron-electron interactions, which have been predicted to generate giant bandgap renormalization (BRN) and excitonic effects. BRN is a shift of interband absorption that is caused by a photon-induced electron-hole plasma (see Figure below).

Lately, layered PtSe$_2$, a Group-10 transition metal dichalcogenide, has been demonstrated to be one of the most promising 2D materials for adoption by industry due to its unprecedented photonic, physical and chemical properties along with low-temperature synthesis methods, high charge-carrier mobilities and long-term air stability. We recently observed very large BRN effects in PtSe$_2$ thin films using optical wavelength-degenerate ultrafast pump-probe experiments. The renormalized bandgap and large exciton binding observed has a range of applications in valleytronics and ultrafast photonics. To quantify BRN in PtSe$_2$ thin films, a quasi-equilibrium carrier distribution model can be employed. This project will extend our computational model to understand and fit experimental results and obtain important material parameters.


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[2] Rate equation simulations of ultrafast population dynamics in large organic molecules and nanostructures

The optical properties of all materials change dramatically when excited by high intensity laser pulses. In large organic molecules such as porphyrins or phthalocyanines, and in large nanostructures such as 2-D nanoplatelets and quasi-1-D nanotubes, these processes generally occur on a picosecond to femtosecond timescale. Rate equations are a suitable mechanism to simulate
the significant excited state population dynamics and to ultimately obtain the intensity dependent optical response. The objective of this project is to numerically solve appropriate partial differential equation system describing these rate equations, and to compare the results with previously published experimental data.

[3] From Purcell (weak) to Rabi (strong) light-matter interaction with coupled 2D materials and nanoantenna

**Supervisor:** Prof. Louise Bradley

Contact Prof. Bradley

Computational

The interaction between light and matter can occur in a strong coupling regime only occurs when certain conditions are met. It fundamentally changes the states of the coupled system. In the past this required optical cavities with very high-quality factors and working at cryogenic temperatures. Strong coupling has recently been observed in the Bradley group at room temperature using nanobipyramids interacting in monolayer MoS$_2$. This project will explore different geometries to optimise and control the strong coupling regime. The project will be a combination of experiment and simulation. The experiments will include dark field scattering and photoluminescence measurements on single nanoantenna. The simulations will be performed using finite difference time domain calculations to explore different structures and materials.


**Supervisor:** Prof. Louise Bradley

Contact Prof. Bradley

Computational

This project will explore tunable metasurfaces based on vanadium dioxide (VO$_2$), a phase change material that can be switched from an insulating to metallic phase both thermally and electrically. The project will involve the growth of VO$_2$ by plasma laser deposition, the fabrication of nanostructures surfaces, and characterisation of the phase change properties of the VO$_2$ and tuning of the metasurface properties via the thermally actuated phase change of the VO$_2$ material. The project will include the development of an experimental test-bed to characterise the optical phase control and anomalous reflection. Complementary simulations to design structures and interpret experimental observations may be performed using finite difference time domain software.
Spintronics deals with the manipulation of spin currents in order to produce a signal, and is widely applied in spinning disk and tape data storage as well as emerging technologies such as spin-torque oscillators and MRAM. Mn$_2$RuGa (MRG) is a promising material for these applications, being a zero-moment half-metal. In order to maximise the signal produced by the tunnel junction where it is deployed during usage, the interface between MRG and the oxide barrier used in a magnetic tunnel junction must be as clean as possible. Any diffusion/oxidation at the interface will interfere with coherent tunnelling, and reduce spin-polarisation of the tunnelling current. One way to inhibit these effects is to introduce a thin dusting layer of another material.

The Trifolium Dubium (TD) deposition and characterisation platform is a new multi-technique thin film system within the Coey/Stamenov group housed within CRANN, incorporating various industry-standard and research-critical physical vapour deposition and analytical techniques. The system is built around a central distribution chamber, allowing for deposition and subsequent surface analysis to be performed without breaking vacuum. A selection of appropriate materials will be used as dusting layers. Using TD, the student will take X-ray photoelectron spectra of the various layers throughout the deposition and annealing process, and analyse to produce an understanding of the interactions between the various layers at each stage. These will be then be correlated with tunnelling characteristics of patterned devices.

Modern thin-film devices require well matched interfaces in order to minimise signal losses, particularly in semiconductor and spintronic applications. Ultraviolet photoelectron spectroscopy (UPS), in particular angular resolved (ARPES), gives information regarding the electronic structure of materials close to the Fermi level. Understanding this structure helps to build models for
The student will utilise TD to measure and analyse X-ray photoelectron and angular resolved UPS spectra of single crystal materials, epitaxially grown sputtered films, and pulsed laser deposited films, with the aim of recovering the unpolarized band dispersions of the conduction band electrons, where possible.

[7] Ultrafast sublattice resolved magnetisation dynamics in ferrimagnets

**Supervisors:** Dr. Jean Besbas and Prof. Michael Coey

Contact Dr. Besbas

**Experimental**

The magneto-optical Kerr effect (MOKE) is widely used to measure the magnetisation with light. In a classic ultrafast magneto-optics experiment, an intense femtosecond pulse of light, the pump, triggers a dynamics of magnetisation that can be subsequently measure with another weak pulse, the probe, through the MOKE. Providing that the pump-probe delay is controlled, such a pump and probe experiment allows measuring the magnetisation dynamics induced by the pump down to the ultrafast sub picosecond timescale. The measurement of the dynamics of the magnetic order in antiferromagnets and ferrimagnets, where respectively two equivalent and inequivalent subsystems have their magnetisations antialigned, is trickier. Indeed, in antiferromagnets, the MOKE of one subsystem exactly compensates the MOKE of the other subsystem leading to the absence of overall MOKE. To circumvent this issue, a second order magneto-optical effect called the magnetic linear birefringence (MLB) can be used. The MLB scales as the square of the magnetisation, making the contributions of the two subsystems equal. The MLB manifests itself as a change of refractive index between in the direction of the magnetisation of the sublattices. In ferrimagnets, the MOKE is the sum of the contributions of two sublattices that is generally non zero. However, the problem lies in the inability to discriminate the magnetisation dynamics of each subsystem individually. To solve that problem, a measurement of the magnetic circular dichroism (MCD) dynamics can complement the measurement of the MOKE dynamics. The MCD causes a linearly polarised light to become elliptically polarised after interaction with the magnetisation. If the sensitivities of the two sublattices to the MOKE and MCD are different, this approach might allow reconstructing the dynamics of each sublattice individually. In this project, we propose to implement MLB and MCD measurements in an optical pump and probe experiment to resolve the sublattice magnetisation dynamics of compensated ferrimagnets. Our team has a longstanding expertise in developing innovative magnetic materials. Therefore, the measurements will be done on ferrimagnets recently developed in our team such as Mn$_2$RuGa or DyCo$_2$. The successful candidate will learn basis in ultrafast optics and advanced polarimetric methods applied to the detection of magnetisation. This project will take place in the photonics laboratory of Trinity College. You are very welcome to contact us for any complementary information or to plan a visit of our facilities.
Calcium carbonate (calcite) is slightly soluble in water, and unlike most other solutes, its solubility decreases as temperature is increased. This causes problems in areas with hard water (> 100 parts per million of dissolved CaCO$_3$) because the calcite precipitates as limescale, and forms an insulating layer encrusting the insides of pipes and surfaces of heating elements when the water is heated. The worldwide economic cost of the limescale problem is estimated to be billions of euros.

It has long been claimed that passing water though a nonuniform magnetic field created by an array of permanent magnets around the pipe alleviates the problem, but these claims were met with scepticism by many physicists because they had no idea how the fleeting magnetic treatment could possibly alter the precipitation calcite that takes place hours later. Only quite recently has evidence for the presence of nanoscale hydrated polymeric clusters of calcium carbonate in water has given rise to new ideas about the influence of singlet/triplet proton pairs on the nucleation of CaCO$_3$ polymorphs (1). The project involves treating hard water with four different commercial magnetic devices in controlled laboratory conditions using a twin-channel peristaltic pump. The water will be characterized by zeta-potential measurements. Limescale formation will be examined using X-ray diffraction and electron microscopy to identify the CaCO$_3$ polymorphs (calcite, aragonite, vaterite) formed in the scale. Based on the results, a new device for magnetic water treatment will be designed.

A publication on earlier study of this topic with an SS project student has been cited 150 times (2).


Water containing bulk nanobubbles with a radius of about 80 nm containing air of another gas can be readily prepared by ultrasonic cavitation. The content is up to $10^9$ bubbles per cm$^3$. Their presence can be detected by laser light scattering and measurements of zeta potential. This nanobubble water is now attracting widespread interest (1) ranging from doctors interested in ultrasonic imaging to farmers interested in washing lettuce or growing marijuana. It is believed that the surface of the bubbles is negatively charged with reactive oxygen species such as OH$^-$ or OH$^·$. However, two big scientific questions remain unanswered (2). Firstly, How can such tiny bubbles be stable? (The Laplace pressure inside in $2\gamma/r$, ($\gamma$ is the surface tension of water, $r$ is the nanobubble radius) or about 15 bar; they should disappear within microseconds and secondly, How can free radicals persist at the surface? They should decay in nanoseconds.
This project involves producing and characterizing nanobubble water by cavitation from water with different hardness (dissolved ion content) and chemical additions such as polar surfactants. Magnetic treatment will also be explored. The water will be characterized by measurements of zeta potential and laser light scattering. Calculations using a new quantum field theory of coherence in water may also be undertaken by a student who likes to explore novel experimentation and advanced theory.

(2) K. Yasui, T. Tuziutti and W Kanematsu, Mysteries of bulk nanobubbles (ultrafine bubbles); stability and radical formation, Ultrasonics Sonochemistry 48 259 (2018)

[10] In-situ imaging of magnetic domains generated by single femtosecond light pulse

Supervisor: Prof. Michael Coey
Contact Prof. Coey
Experimental

To reduce the magnetostatic energy, the magnetisation tends to form multiple non-collinear magnetic domains of uniform magnetisation on the microscopic scale. In thin films, these magnetic domains can readily be visualized exploiting the magneto-optical Kerr effect (MOKE) in a microscope. Surprisingly, little is known on the formation of magnetic domains under femtosecond light pulse irradiation although it is well established that the short duration and high peak power of femtosecond pulses can trigger a variety of out-of-equilibrium magnetisation dynamics such as, for instance, sub picosecond demagnetisation, magnetic ultrafast toggle switching of magnetic domains or ferromagnetic mode excitation. To develop our understanding of the action of a pulse on magnetic materials, we are building a MOKE microscope with in-situ access for femtosecond pulses in the photonics laboratory of Trinity College. In that context, we are looking for a motivated candidate in experimental physics to contribute to the development of the tool and perform measurements. The versatility of this project can accommodate a variety of approaches that would fit with various candidates. One approach could focus on the development of the tool i.e. addressing the control of the pulse distribution, energy, and polarisation, optimizing the contrast of the microscope, integrating temperature control of the sample and magnetic field capabilities. Another approach would be to use the microscope as such and profit of the expertise of our team in magnetism to do an unique and impactful comparative study of the characteristics of optically generated magnetic domains in a variety of magnetic thin layers. We are especially interested in the formation of magnetic domains when the pulse power density on the sample yields an ultrafast heating of the magnetic system in the vicinity of the Curie temperature. As such, measuring magnetic domain formation with respect to the sample temperature and pulse energy in at least one sample will be a requirement for a successful project. To each student, our team provides support and expertise in the domain of magnetism and fast optics in a friendly environment that we believe necessary for the growth of science. As such, you are very welcome to contact us for any complementary information or to plan a visit of our facilities.
[11] Printed supercapacitors from graphene and boron nitride nanosheets

**Supervisor:** Prof. Jonathan Coleman  
**Contact Prof. Coleman**

**Experimental**

The ability to print electronic or energy storing devices using nanomaterials is an important part of nanotechnology. Supercapacitors are energy storage devices consisting of a pair of electrodes resembling a capacitor. However, the dielectric layer between the electrodes is replaced by an electrolyte. Application of a voltage causes oppositely charged ions to move to each electrode/electrolyte interface where they are balanced by layers of charge on the electrode. This arrangement allows the storage of energy at much higher density than in traditional capacitors. This energy density can be boosted even further by using nanomaterials such as graphene or nanotubes to make very high surface area electrodes. However, one problem is low cost supercap fabrication while another is containment of the electrolyte. This project will explore ways to print supercapacitors by printing a network of graphene nanosheets as a bottom electrode followed by a layer of (insulating) Boron Nitride (BN) nanosheets as a spacer followed by another network of graphene nanosheets as a top electrode. Here the BN network is highly porous and can act to contain the electrolyte. The project will study the properties of the resultant supercapacitors as the thickness of both graphene electrodes and BN spacer are varied, focusing on energy density and power delivery.


**Supervisors:** Dr. Majid Fazeli Jadidi and Prof. Graham Cross  
**Contact Dr. Jadidi**

**Experimental**

Two-dimensional materials are among the most promising materials for use in future nanotechnology due to their novel mechanical and electronic properties. Graphene as a well-known 2D material has attracted intense attention of researchers mostly because of its unique electronic, mechanical characteristics such as giant charge carrier mobility, a strange quantum Hall effect, superlubricious vanishing of friction, etc. Self-assembly of graphene ribbons is an unusual and an exceptional behaviour discovered at TCD (1) with similarities to origami-like paper folding. In this project, you will investigate whether graphene self-assembly is a phenomena occurring in the general class of 2D materials. You will investigate the preparation of MoS$_2$ flakes by mechanical exfoliation and mechanical characterization of self-assembling ribbons in these and CVD-grown MoS$_2$ flakes with atomic force microscopy (AFM).

Optically detected magnetic resonance of diamond nitrogen-vacancy centers

Supervisors: Dr. Majid Fazeli Jadidi and Prof. Graham Cross

Experimental

Have you heard about colour centers in the diamond lattice? These are a kind of point defect in the diamond lattice with unique optical and magnetic properties that make them one of the most promising candidates to be employed as quantum sensing elements in the atomic scale. As the name suggests, they also are responsible for the colour seen in some diamonds! How they can be formed? A missing carbon atom from one of the lattice sites is called a "vacancy". When a nitrogen atom N, which substitutes for a carbon atom, takes place in the vicinity of a lattice vacancy makes a pair known as nitrogen-vacancy (NV) center. NV centers can be created in the diamond containing nitrogen with different techniques such as irradiation with electrons, neutrons and high energy ions. NV colour centers can be formed in two different charge states; neutral and negative. Both types of NV centers have photoluminescence property, however, the negatively charged one with spin-state-dependent photoluminescence intensity can be manipulated and optically readout at room temperature. It has been considered as an efficient sensor for detecting magnetic fields, electric fields, temperature, and pressure.

How they can be used as quantum sensors? The NV centers with negative charge state have the characteristic zero phonon line (ZPL) fluorescence at 638 nm. This "zero phonon line" refers to the electronic transition from the excited state to the ground state. They can be excited with a laser beam below this wavelength resulting in spin-state dependent photoluminescence intensity. An external static magnetic field results in sharp resonances in the intensity and wavelength of the photoluminescence that can be optically detected. The resonance frequencies are well-characterized functions of the magnetic field B, electric field E and temperature T. The optically detected magnetic resonance (ODMR) is a detection instrument to obtain the spin resonance spectrum of NV centers. The spin resonance spectrum is collected by monitoring the photoluminescence intensity while sweeping the microwave frequency.

In this project you will investigate the operation of simple diamond NV center fluorescence detection setup and see if it can be used to measure temperature.
Semiconductor lasers have a tunable emission due to the dependence of the refractive index of the materials in the laser diode on temperature and on carrier density. While temperature generally produces a red shift in wavelength, carrier density effects produce a blue-shift. In this project, we will investigate these effects in a novel device structure developed by the Photonics group in TCD. These lasers will be studied to see the effects of changing the cavity length on the emission and how the grating structure is used to produce emission across 30 nm or more centered around 1310 nm. This project is mostly based in the laboratory but will also have some component of modelling so that the students understand how to design a semiconductor laser for a particular application in mind. Laser that emit around 1310 nm will have applications in optical communications systems for uplink from users to the network core. You can see further background information here.

The wavelengths of semiconductor lasers generally change with changing temperature since the refractive index of most common materials depend on temperature. In many applications, the temperature of these lasers must be carefully controlled using a thermo-electric controller. For certain applications it is desirable to have lasers operate with such controllers while still maintaining a central frequency that does not vary by more than +/- 0.5 GHz over a temperature range of 100°C. Athermalisation refers to the process by which currents are varied to different sections of a laser so that its internal temperature does not vary as the ambient temperature does. We will investigate the processes for athermalisation of lasers that operate at the 1.5 and 1.3 micron optical communications bands and how we different cavity lengths affect the athermalisation. We will also investigate how the different numbers of contacts on the device can assist in improving the athermalisation. You can see further background information here.
Machine Learning of Gas Turbine Energy Conversion Physics

**Supervisor:** Prof. Stephen Dooley

This is an opportunity to be involved in an exciting international collaboration between Siemens Industrial Power Generation business units across Europe and North America, lead by Siemens Power Generation Canada, and Trinity College Dublin. Gas Turbines account for 35% of global electricity generation. This share will expand over the coming fifty years as wind and solar electricity technologies build grid capacity, due to the unique ability of the gas turbine to rapidly and dynamically balance grid load due to the intermittency of renewables. With the goal to reduce global carbon dioxide production while increasing electricity generation, gas turbine combustor design must advance to increased efficiency and to the clean burning of a wider range of renewable gaseous and liquid fuels. To do this, faster and more accurate fluid-chemical reaction numerical models are needed for computational fluid dynamics orientated machine design. This project applies and develops machine learning methods to the design and construction of highly accurate and minimally detailed numerical models that accurately implement all the important physics (Navier-Stokes, Molecular Thermodynamics) and chemistry (Collisional and Transition State Theory) needed to describe the flow-chemistry interaction of the gas turbine oxidation of several renewable fuels in the actual gas turbine combustor geometry. The key task is the dimensional reduction of the myriad of detailed physics models needed to describe these interactions, into reduced analytical representations. Machine-learned model reduction analysis will identify which authentic physical terms must be reduced. The definition and testing of several objective error functions will form the basis for unsupervised machine learning. Inaccuracies in the reduction will then be compensated for by evaluation of the hundreds of thousands of objective error functions generated by Machine-learned Monte-Carlo and Genetic Algorithm driven unsupervised optimizations of the reduced model terms. Specifically, the student will exercise and advance the Adaptive Monte Carlo Optimization for Combustion Kinetics (AMOCK) method developed by TCD Energy Research. This is implemented in Python with the main numerical computations performed on a CANTERA engine. Python, high performance computing, excel based numerical analysis and data presentation, are all key skills that will be developed in the student through this project. Training in the scientific knowledge of data science, machine learning, combustion physics, reaction kinetics and energy science will be accrued, in addition to general scientific training.

Data Mining and Principal Component Analyses of Rapid Compression Machine Ignition Physics

**Supervisor:** Prof. Stephen Dooley

This is an opportunity to be involved in a 34 University international collaboration across Asia, Europe and North America, which aims to understand the essential fluid dynamic, chemical reaction kinetic, and thermodynamic factors that control ignition in reciprocating engines. Ignition is the spontaneous process whereby fuel/oxidizer converts to a set of reaction products of lower free energy than reactants in a rapid hugely exothermic process. The operation of efficient novel energy conversion concepts depend on precise knowledge of this ignition process. However,
obtaining this is a difficult task, as (i) the time taken for ignition to occur varies from the millisecond to few nano-second time-scale depending on the energetic state of the process, and on (ii) the multiple-time scales of the reacting phenomena means that it is not possible to separate the chemical reaction component of the ignition event, from heat transfer and fluid dynamic mixing components in measurement. This complexity creates a problem whereby the instruments built to study the ignition phenomena have the effect of interfering with the intended measurement in a manner specific to the design particularities of each device. To make progress on the matter of understanding ignition, it is thus necessary to know how each design component of each device influences the ignition process. To achieve this goal the Trinity Energy Research Group have designed a coordinated an international measurement campaign across 34 Rapid Compression Machine facilities used to measure ignition. Each facility has performed ignition measurements at the "same" precise conditions. After three years of work, all the data is now collected and is being processed. The Senior Sophister research project involves the implementation and development of data science learning algorithms to process the library of ignition measurements, and to relate their dynamic behaviour to the collected device design variables through a Principal Component Analysis. The PCA will be supported by detailed information from a set of idealised physics simulations where corrupting fluid mechanic effects will be parameterised with scientific rigour. The findings of the study must be reported by a peer-reviewed publication before January 2021, the involved students will be expected to contribute toward this effort, and will be given every opportunity to earn the merit of their name on a peer-reviewed publication as an undergraduate. The data science component is implemented in Python/Matlab and the idealised fluid dynamic reacting simulations performed on a CANtera engine. Python, high performance computing, excel-based numerical analysis and data presentation, are all key skills that will be developed in the student through this project. Training in the scientific knowledge of data science, machine learning, combustion physics, reaction kinetics and energy science will be accrued, in addition to general scientific training.
Spin transport in organic materials

Supervisor: Dr. Andrea Droghetti
Contact Dr. Droghetti

Computational
Can be done remotely

Organic materials, such as molecular crystals and polymers, are generally considered ideal media for spin transport owing to their long spin-relaxation time. However, experiments have reported contradictory results and the physics underlying these materials is still poorly understood. Charge and spin-transport in organic materials has been theoretically described in terms of "two fluids" (1,2). The charge current is due to electrons hopping between molecular units or impurities. Concurrently, unpaired electrons can be trapped at molecular units/impurity sites, which therefore present magnetic moments. The spin current is eventually enabled by the exchange coupling between these magnetic moments and is carried by spin-waves. Charge and spin propagate through different regions of an organic material as two fluids with different diffusion constants. Recent experiments claimed some evidence for this two-fluid behaviour (3,4).

In this project we will construct a computational multiscale approach to simulate charge and spin-transport in organics. The goal is understand how the two fluids emerge in some real materials and what the key material properties affecting spin transport are. Ultimately, we aim to introduce conceptually new ways to enhance the spin current in organics. To begin with, we will model some of the typical devices used in experiments and we will obtain the model parameters via first-principles electronic structure calculations (5). Then, transport will be addressed either by means of the kinetic Monte Carlo technique or by solving the quantum master equation. Finally we will extend our approach to account for the interaction between electrons and photons in a new type of devices, where an organic material is encapsulated inside a plasmonic nanostructure. A recent experiment reported that the charge current in these devices was drastically enhanced because of the very strong electron-photon coupling and the formation of polaritonic states (6). We will predict here whether the spin-current can be increased in a similar way.

(3) S. J. Wang et al., Nat. Electron. 2, 98 (2019)
Anyone involved in studying the transport properties of quantum systems acknowledges that it is straightforward to calculate the conductance of a device once all its scattering centres are fully located and specified. However, it is enormously challenging to perform the same task in reverse, i.e., to find information about the composition of scatterers in a quantum device from its conductance alone. This type of challenge is what is known as inverse problems, which is the process of obtaining from a set of observations the causal factors that generated them in the first place. While there are numerous examples of inverse problems in classical physics, they are a lot scarcer in the quantum realm, particularly if the problem in question involves heavily disordered environments. In this project you will attempt to develop an inversion tool capable of extracting compositional information from a (disordered) quantum device by looking at its conductance signatures. This project requires good understanding of Quantum Mechanics and excellent problem-solving skills. Project involves analytical and computational abilities in equal measure.
Steady-state thermodynamics of composite collision models

Supervisors: Dr. Giacomo Guarnieri and Prof. John Goold

Computational

Abstract — Quantum Thermodynamics is the fascinating branch of Physics that aims at characterising energy exchanges, in the form of work and heat, between quantum systems. These studies pave the way to exploit the peculiarities of the laws of quantum mechanics to realise efficient next generation quantum technologies. While exquisite experimental control of quantum systems has been achieved to date, their unavoidable interaction with a surrounding bath has usually detrimental effects on their genuinely quantum properties, notably coherence and quantum correlations. The framework of open quantum systems allows to account for these environmental effects through methods and models that provide a very accurate description of the system’s evolution. A particularly useful one is given by the so-called quantum collision models, which constitute a very rich platform to simulate open quantum systems in a simple yet reliable and highly flexible way. In this theoretical and numerical project, we will continue the investigation the steady-state thermodynamic properties of collision models started recently in G. Guarnieri, et al. arXiv:2001.01723v1, by considering a composite two-qubit system. This would open the possibility to achieve steady-state with entanglement or other forms of quantum correlations and characterise on one hand the energetic cost of creating and maintaining such state, and on the other hand the extractable work from purely quantum resources. Another aim will be to identify contributions to the thermodynamic currents, which sustain the above mentioned quantum correlations.

Fig.1 Schematic representation of collision models: a system made of two qubits sequentially interacts with an ancillary system for a given time and then move on to interact with the next one. After many collisions have taken place, the system will reach a stable configuration where properties of the system will not change but currents of heat and work will continuously flow between the system and the ancillae.

Profile — This project will provide the student with the unique opportunity to approach open quantum systems theory with little background knowledge, thanks to the clear and practical analysis offered by collision models. As a result, the student will learn fundamental and ubiquitous concepts of quantum physics such as qubit and qubit gates. Moreover, the results achieved through this project are novel, thus representing genuine research which can be in principle lead to publication in peer-reviewed journals. Furthermore, the student will learn how to simulate simple quantum systems through Mathematica software, which represents a widely employed and useful research tool. Instructive codes will be provided throughout the project.

Many-body localized dynamics

**Supervisors:** Dr. Francesca Pietracaprina and Prof. John Goold

**Contact Dr. Pietracaprina**

Computational

**Abstract** - Quantum dynamics in the presence of disorder shows surprising features. Among those, a phenomenon called many-body localization is arguably the most striking one. In highly disordered quantum materials, transport and thermalization is surprisingly absent; a highly disordered, isolated, strongly interacting system, prepared in a non-equilibrium initial state, will not reach thermal equilibrium. This is of fundamental importance to our theoretical understanding of out-of-equilibrium properties of systems with impurities and disorder.

In this theoretical and numerical project, we will investigate a model that has a many-body localization-delocalization transition in a configuration very close to an experimental setup, looking at the dynamical entanglement properties across the phase transition. The aim of the project is to identify the transition point and a set of parameters useful for a comparison with an upcoming experiment.

**Figure 1:** Sketch of the phenomenology in a many-body localizable model. In the MBL phase, a state has support in a finite fraction of the total available Hilbert space $\mathcal{H}$ and is quantum non-ergodic. Moreover, the state retains local memory of its initial state (a charge density wave state in this figure) at long times.

**Profile** - Throughout the project, the student will have the opportunity to learn about out-of-equilibrium dynamics of quantum systems and disordered systems. Given the type of project, the student should have a very good theoretical understanding of quantum mechanics, mathematical skills and programming abilities. Some computer codes in Python or C++ will be provided.

**References** - F. Anza, F. Pietracaprina, J. Goold. Quantum 4 250 (2020) [https://doi.org/10.22331/q-2020-04-02-250](https://doi.org/10.22331/q-2020-04-02-250)

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Quantum dynamics of an impurity in a cold fermionic gas

**Supervisors:** Dr. Mark Mitchison and Prof. John Goold

**Contact Dr. Mitchison**

Computational

The lowest temperatures in the known Universe are now routinely created and studied in Earth-bound laboratories. Rarefied, ultracold gases of atoms are controlled quantum systems that can be used to simulate complex quantum many-body phenomena in condensed-matter or high-energy physics and beyond. This project will study the behaviour of an impurity atom of a different species that is plunged into the ultracold gas. Using a combination of analytical and numerical methods, you will explore how the time evolution of the impurity’s quantum state is affected by collisions with the surrounding gas atoms. In particular, you will investigate how...
things change as the position of the impurity is varied through the gas. The project will deepen your understanding of the emergence of irreversible behaviour in many-body quantum systems.
The presence of viral proteins or immune responses to virus in biological fluids can be quantitatively analysed using nanomechanical resonators. Native individual molecules/receptors are anchored to the surface of micron scaled cantilevers that are immersed in liquids. The anchoring to the interface is usually provided using either biomolecular recognition, or covalent immobilisation. We will explore both protocols to evaluate conformational integrity and compare to existing protocols like enzyme linked immunosorbent assays (ELISA). Nanomechanical diagnostics provides a single step quantitative label-free approach in contrast to conventional assays that require multiple steps with larger sample volumes and labelling of the involved entities. The quantity of the specifically bound biomolecules can be evaluated by correlating the shifts in resonance frequency and quality factors of sensors that are measured in real-time in volumes of a few microliters. The selectivity of the assay relies on the differential read-out of sensors responses on an array of cantilevers oscillating in fluids.

In particular the students will:

1. Learn how to prepare and activate MEMS silicon structures to specifically bind biomolecules in liquids.
2. Develop a protocol for corona virus related molecules and compare to current protocols applying biomolecular recognition (ELISA)
3. Operate a diagnostic MEMS platform to measure molecular binding by tracking sensor oscillations with PLL feedback in liquids
4. Measure quantitative/qualitative nanomechanical responses in fluids using MEMS technology.
Single Photons in the Vicinity of an Optical Black Hole

Supervisor: Prof. Ortwin Hess
Contact Prof. Hess
Computational

Background: For the past three decades, optical quantum technologies have been based on high-finesse cavity (e.g. a pair of mirrors). An atom inside the cavity could then interact with the same photon multiple times, as the light bounces back and forth between cavity walls before eventually escaping into free space. This mechanism is at the basis of the strong coupling regime, whose rich phenomenology greatly advanced our understanding of quantised radiation. Unfortunately, however, these all required cryogenic temperatures and were thus not very practical for quantum technologies. Recent new exciting possibilities for strong coupling and light-matter interaction are emerging beyond the traditional cavity QED scenario. Following recent advances in the design of stopped-light structures [3] and realisation on the nanoscale (see, for example, our recent review paper in Science [2]), it is now possible to devise media with an ‘optical black hole’ (a singularity in the density of states) in whose vicinity the group velocity of light is negligible for a wide range of wavevectors [3]. Such media allow for new physics with non-trivial interactions between photons and atoms: if emitted photons cannot propagate away from their source atom fast enough, they can have a significant chance of being re-absorbed and re-emitted multiple times before escaping. Such dynamics would be reminiscent of the strong coupling regime of cavity QED, despite the absence of a cavity! Concurrently, there are opportunities involving nanoscale plasmonic structures which have recently elevated strong coupling to the practically relevant room-temperature regime [4].

SS Project: We shall start with a familiarisation about the basics of ultrashort light on the nanoscale (as discussed e.g. in our recent review paper in Science [2]) and nanoscale optical strong coupling [4] as well as with standard techniques of quantum optics and the theory of open quantum systems models [5]. As a stopped-light singularity represents a setting beyond the standard framework of Lindblad master equations you will subsequently look at extending this theory and also use a recently established computational approach to describe single-photon emission from quantum emitters [6].

REFERENCES
Winner-loser models aim to describe the formation of hierarchies in societies as a consequence of pairwise interactions (fights) between individual agents. This project implements various fighting rules in agent-based computer simulations to determine the resulting stationary status distributions which characterize societies.


Buckling of a linear chain of hard and soft spheres (ball-bearings, soap bubbles) in a confining potential

Spheres (ball-bearings, soap bubbles) are confined in the lateral direction between opposing hard walls while also being confined in the transverse direction by a harmonic potential. The linear chain is unstable under compression and forms a range of buckled zigzag structures with increasing compression. A number of experimental, numerical and theoretical results exist for such structures. This project concerns numerical solutions for a variety of different boundary conditions, with possibly also some experimental data analysis. The work will be carried out in collaboration with a PhD student.


In the scanning transmission electron microscope (STEM), the video frame rate is typically around one or two frames per second. This is too slow to capture fast dynamic events such as those in in-situ microscopy. At these frame-rates, and with the frame only updating line-by-line, a common artefact called rolling shutter distortion can occur, the same as can be seen with TV cameras. Alternatively, image interlacing (a technology from high-definition TV) can be used. This is where only the odd scan lines are captured one frame, and even the next. This doubles the frame rate at the expense of having only half the detail in each frame, where now moving objects may appear torn on alternate lines. Deinterlacing techniques can be used to mitigate the negative aspects of interlaced video capture by reducing image artefacts while retaining the frame rate boost. The goal of this project is to determine if these techniques are also applicable to STEM.

Using video-game GPUs to better predict focus-blur in the Transmission Electron Microscope

Scanning Transmission Electron Microscopy (STEM) is an invaluable tool in modern materials science and nanotechnology. The performance of these instruments depends on many factors, including importantly the quality of the electron lenses. Defects in these lenses can introduce both spherical aberrations (Cs) and chromatic aberrations (Cc) in the final image and reduce the ultimate resolution. When planning experiments, it is often useful to simulate in advance the image performance that we might expect (including imperfections and aberrations like the defocus and the spherical aberration). These simulations can be calculated using computer software such as Prismatic (1). Currently, this software does not include the effects of chromatic aberration, though it has been shown that this can be approximated by hand by performing a weighted-average sum for various defocus values (2). This project aims to implement the Cc contribution in the Prismatic software automatically without the need for tedious manual calculation. This will enable nanotechnology experiments to be designed faster and more reliably. Potentially we will evaluate the use of PC graphics cards (GPUs) to accelerate the calculation.

Optimized antireflection coatings for Rooftop Solar PV

Supervisor: Prof. David McCloskey
Contact Prof. McCloskey
Experimental
Back

Aim: To develop antireflection coatings specifically for rooftop solar PV.

Background: Developments in the solar power industry over the past 50 years have led to improvements in both efficiency and economic viability of solar power installations. The cost of photovoltaic solar panels for example has dropped from an average of 76.67 USD/Watt in 1977 to 0.37 USD/Watt in 2017. Large Scale solar PV is now becoming competitive with other renewable technologies such as offshore wind even in Ireland. The optimum mounting angle for fixed angle mounted solar PV depends on the latitude, but is around 45 degrees in Ireland for single panel strings. The panels themselves should face almost directly South. When multiple strings are installed we must consider the string to string shading and the total available site area. Large scale industrial solar installations are often placed on flat roofs where a space is at a premium. It is not practical to mount solar panels at high angles on due to excessive wind loading so they are often mounted in landscape format and at a maximum of 10°. A recent trend has seen a preference for mounting panels in East-West orientation at 10°. This maximises the number of panels that can be fit on a fixed size flat roof, however these panels will not be operating under optimum illumination.

![Image: 70MW solar farm in PEG, India, built and operated by Phelan Energy group.](image)

Project description: In this project the student will investigate a number of antireflection concepts that will improve solar panel performance when mounted at low angle in East-West orientation. First these coatings will be modelled numerically, and then time and lab access permitting we will make some prototypes for demonstration. These designs will be tested using lab scale tests, but also could be tested on our full scale outdoor test site.

Learning outcomes:
Student will learn:
- Numerical modelling techniques for optical problems.
- Modern solar cell designs and trends.
- Thin film deposition techniques.
- Solar panel setup.
- Solar simulator testing.

Companies operating in this area in Ireland:
Modelling of Thermal performance of Floating Solar Photovoltaics

Supervisor: Prof. David McCloskey

Contact Prof. McCloskey

Experimental

Aims: to understand performance limits of floating solar PV

Background: Floating photovoltaic (FPV) is an emerging spin on conventional Photovoltaic which uses interlocking floating panel supports to create a large floating platform of Solar PV, such as shown in Fig 1. These can be anchored or tethered to the surrounding bank.

![Figure 1](image1.png)

**Figure 1** (a) The floating solar farm in Huainan, China is made up of 350,000 panels and takes up 800,000 square meters. (b) The Seabrook FPV installation in the Netherlands, with a yearly energy yield of 13.33 MWhr, saving over 6500 tons of CO₂ emissions a year.

This technology has a number of advantages over conventional land or rooftop mounted solar PV. This includes, no land occupancy, easy installation and decommissioning, reduction in water evaporation, module cooling, easier tracking, and environmental control (reduction in algae bloom). At the beginning of 2018, some 60 floating solar farms of over 1 MW had been installed around the world. Their combined capacity was still very small, totalling less than 200 MW (the equivalent of a large land-based solar farm – enough to provide energy to around 200,000 people). However, this figure has more than doubled over the course of a year. Japan, where farm irrigation reservoirs are plentiful and land is expensive, naturally became a pioneer in floating solar technology and is still leading the industry. The farms can be built on sites of various sizes, such as impoundments, quarry lakes, farm irrigation and industrial water reservoirs, water treatment facilities and flood plains. By the end of 2019, the cumulative global installed floating solar capacity was expected to reach a minimum of 2.4 GW which would be enough to satisfy just under 1% of annual global solar demand. Moving ahead between 2019 through 2024 demand for this technology is likely to grow by an average of 23% YoY, which will bring costs down significantly.

Project Description: In this project the student will investigate a novel FPV design which will optimize the thermal performance of FPV while at the same time providing stability against high winds and rough waters. The project will use numerical modelling of heat transfer and fluid dynamics, but if the opportunity exists we can also do some scaled down lab experiments and outdoor testing.

Learning outcomes: Student will learn:
- Solar simulator testing
- Modelling of heat transfer
- Modelling of fluid dynamics.
Modelling of novel heat exchanger for Solar Thermal Applications

Supervisor: Prof. David McCloskey

Aim: To develop and test novel heat exchanger designs to improve performance of solar thermal energy collectors.

Background: Residential energy demand in Ireland has been increasing since 2014, and accounts for around a quarter of Ireland's overall energy demand. Of that demand, the SEAI estimate that 19% of household energy consumption is for water heating. Solar thermal technology uses energy from sunlight to generate heat which can be used as hot water for residential and industrial applications or for space heating. Conventional solar thermal systems come in flat panel or tube designs (Fig.1). Key components of these structures are the solar selective absorber surface, and the thermal insulation design. The solar absorber in the material or paint which generates heat, and the thermal insulation ensures that this heat results in a high temperature rise. This temperature is then used as the hot bath in a heat exchanger system. The higher this temperature the more efficient the heat exchange process.

![Figure 1](image)

Figure 1: (a) Flat plate solar thermal design; (b) Solar thermal tube collector array; (c) Cross-sectional diagram of solar thermal tube with copper heat pipe collector.

Project Description: In this project the student will investigate a novel heat exchanger design recently patented by Prof. McCloskey’s research group and its application to Solar thermal. This heat exchanger could reduce considerably the cost of solar thermal collectors making them a more economically viable option for materials for solar thermal applications. Currently payback periods for solar thermal in Ireland range between 14-48 years depending on technology and deployment. This work aims to reduce the payback period to 5 years making solar thermal a logical choice for reducing residential and commercial water heating as a load on our energy supplies. The project can be performed fully numerically, however if COVID restrictions have been removed the results can be tested in lab and outdoor test site conditions.

Learning outcomes:

Student will learn:

- Solar simulator testing
- Solar thermal technologies.
- Optical and thermal modelling.

Companies in this area in Ireland: Kingspan, Glen Dimplex
Simulation of electronic structure, scanning tunnelling microscopy and spectroscopy of new porphyrin-derived on-surface synthesized porphyrin nanoribbons

Supervisor: Prof. Cormac McGuinness
Contact Prof. McGuinness
Computational
Back

Porphyrin nanoribbons can be formed through on-surface synthesis of porphyrin-derived halogenated precursors by temperature driven dehalogenation followed by covalent coupling. This project will use appropriate density functional theory (DFT) codes to simulate the electronic structure of new transition metal porphyrin-derived template precursor molecules for the on-surface synthesis of existing and new porphyrin-derived nanoribbons. One form of porphyrin nanoribbons has already been synthesised and observed on-surface with scanning tunnelling microscopy (STM), and the formation of these nanoribbons will soon be observed with high-resolution synchrotron radiation-based x-ray spectroscopic methods such as core-level x-ray photoemission spectroscopy (XPS) and x-rays absorption spectroscopy (NEXAFS). Examples of this are shown in the figure below.

![Diagram of porphyrin nanoribbons](image)

**Figure 1:** (a-c) How a di-bromophenyl porphyrin molecule can with temperature dehalogenate (a); couple into a chain (b) and then internally become a ribbon (c) with increasing surface temperature. Observations via STM are shown in (d) and (e) showing cyanin chains and cyanin nanoribbons.

Porphyrins are organic molecules which accommodate a large range of divalent metal ions at the center of the porphyrin structure (macrocycle) giving differing band-gaps and optical spectra via metal ions such as Zn, Ni, Fe, Mn, Cr and Mg, and give rise to e.g. heme and chlorophyll. Halogenated tetra-phenyl porphyrins are ideal as 2D network building blocks. In the system shown, and other more complex precursors, the electronic structure of a single molecule will be calculated to theoretically simulated experimental data. In particular, core level binding energies measured in core level x-ray photoemission (XPS), and densities of states (DOS) which give experimental STM images, as well as the unoccupied electronic structure as measured by x-ray absorption or near edge x-ray absorption fine structure (NEXAFS). The porphyrin chain and subsequent nanoribbon will then be studied through similar simulations and through both lightweight and computationally intensive methods.

Physical insight, experience with unix/linux, some programming or scripting ability and careful thought will be required for this project.

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X-ray magnetic circular dichroism (XMCD) is a synchrotron radiation based x-ray spectroscopy used to measure the magnetic moments and probe magnetic behaviour of materials on an elementally selective basis due to the distinct binding energies of the orbitals probed to connect with the magnetically polarised unoccupied states. XMCD uses circularly polarised x-rays where differential x-ray absorption of a material in a magnetic field is measured in four differing modes: $\sigma^+B^+ = \sigma^-B^+$, $\sigma^+B^- = \sigma^-B^-$ - corresponding to the two differing circular polarizations available ($\sigma^+,\sigma^-$) and the differing applied fields parallel ($B^+$) or anti-parallel ($B^-$) to the direction of propagation of the x-rays. The XMCD spectrum is computed from the difference of any pair of the x-ray absorption spectra. For bulk materials where the underlying x-ray absorption signal is strong, the XMCD is not susceptible to transient problems related to the measurement. However in the case of very small x-ray absorption signals due to small amounts of material, e.g. sub-monolayer coverages of the material being probed, transient problems (noise as well as differing spectral backgrounds due to variable flux from the x-ray monochromator or machine issues) from each separate measurement have an untoward effect on the ability to compute XMCD. This project envisages the development of a robust self-consistent data analysis method whereby a quartet of spectra (or octet of spectra), known to be probing the same amount of material, are treated to obtain reliable XMCD spectra. XMCD data previously obtained at synchrotrons in Sweden (MAX-lab) and the US (ALS) are available for this project. This data arises from gold-capped cobalt nanowire arrays self-assembled on vicinal regularly stepped platinum substrates such as Au(4-7ML)/Co(0.39-0.78ML)/Pt(997) investigated by us in the recent past [1,2]. In brief these samples are parallel arrays of cobalt nanowires whose width vary from 1-atom wide to 4-atom wide, all of which are 1-atom high, and which are spaced 2nm apart on a stepped platinum crystal which acts as the substrate for the self-assembly. The magnetic properties of these cobalt wires change dramatically by the capping with a gold overlay of between 4 to 8 monolayers thickness.

Theoretical simulation of x-ray absorption and resonant inelastic x-ray scattering in transition metal oxides

Supervisor: Prof. Cormac McGuinness

The spectroscopic technique of resonant inelastic x-ray scattering (RIXS) is both a probe of low energy electronic excitations in materials and is sensitive to the electronic structure and chemical bonding of the intermediate state in the scattering thus determining the final scattered spectrum. In rutile metal oxides, such as the prototypical TiO$_2$ or the half-metallic CrO$_2$, the anisotropic bonding of the oxygen anion results in an observed polarisation dependent or natural linear dichroism in the oxygen anion K-edge 1s-2p x-ray absorption spectroscopy (XAS). This can be exploited via polarization and scattering geometry dependent RIXS to decipher details of the occupied and unoccupied electronic structure in these materials to observe the x-ray emission spectroscopy (XES) due to oxygen 2p-1s emission from the occupied valence band. The object of this project is to use existing density functional theory (DFT) codes which simulate the occupied and unoccupied electronic structure and bandstructure of a material via an approximation to the one-step Kramers-Heisenberg equation to properly simulate the RIXS or bandstructure dependent resonant x-ray emission spectroscopy (RXES) observable at the oxygen anion K-edge in synchrotron radiation based experiments. Simulations will first be compared to data obtained from either CrO$_2$, RuO$_2$ or TiO$_2$ and applied to yet to be measured, structurally similar oxides such as rutile OsO$_2$ and MoO$_2$, CoF$_2$, or the antirutile TiN.

Further work would either to simulate the metal L-edge 2p-3d x-ray absorption spectroscopy (XAS) spectrum and the subsequent 2p-3d and 2p-3s RIXS spectra of TiO$_2$ and of CrO$_2$. Or participate in some data analysis of the most recent experimental O K-edge RIXS spectra of RuO$_2$ and CrO$_2$. The nature of the metal L-edge RIXS calculations involves applying an atomic multiplet model to the 2p$^6$3d$^1$-2p$^5$3d$^{1+}$ transition and taking into account solid state effects such as crystal field interactions with the oxygen ligands of the metal ion and also charge transfer between the surrounding ligands and the metal ion. For this latter part a familiarity with programming in a Unix environment would be beneficial.
The packing structure of disordered platelet suspensions

**Supervisor:** Prof. Matthias Moebius
**Experimental**

Microscopic platelet particles, sometimes referred to as 2D nanomaterials or nanosheets, naturally occur in clays, for example. More recently 2D nanoparticles such as graphene and many others can be produced. Suspensions of these nano-sheets are often used to make films for battery electrodes or can be used as fillers to enhance the mechanical properties in nanocomposites. One important quantity is the volume fraction at which these particles form a stress bearing network and its dependence on particle aspect ratio. You will investigate this experimentally by studying a system of macroscopic sheets suspended in a fluid and compare your results with theoretical predictions. This experiment could be done from home. This involves making particles from sheets, weighing them and measure their packing properties using basic measuring tools (ruler, balance, cutter) which would be provided.

**[36] Splashing droplets**

**Supervisor:** Prof. Matthias Moebius
**Experimental**

The splashing of liquid droplets on a solid, smooth surface is a complex physical process that not only depends on the properties of the liquid, but also on the surface roughness and ambient air pressure. Beyond a critical impact velocity, droplets not only spread on the surface but splash and eject tiny droplets. This is important in the context of printed electronics, for example, since splashing reduces the resolution of the printed patterns. In this project you will numerically solve a recent model that predicts the critical impact velocity of droplets in terms of the relevant fluid parameters. You will compare your findings with high speed imaging of droplet impacts. In case of lockdown, the experimental part can be done partially at home without high speed imaging, by using coloured liquid and a paper splash guard that indicates whether splashing has occurred.

**[37] Testing a new fast method for predicting the gap of metal oxides**

**Supervisor:** Prof. David O'Regan
**Computational**

In this recent manuscript we describe in detail a relatively fast, self-contained new method for correcting approximate density-functional theory, which predicts the band-gap of two phases of TiO$_2$ to remarkably high accuracy. This is a long-standing challenge in the area, and if it works only for TiO$_2$ (a p→d charge-transfer case) it is already useful. We would very much like to know the same technique can work as well for other classes of metal oxides, and testing the d→p case is the focus of this project. The student on this project will need to undertake an independent literature review and take responsibility for their oxide material, take responsibility and monitor daily their own calculations, and maintain sound scientific record keeping. In this way they will learn hands-on how the literature review, calculations, visualisation, and interpretation of an applied-DFT study are done.
Simulation of Stokes shifts in light emission by organic materials

**Supervisor:** Prof. Charles Patterson
**Contact Prof. Patterson**

**Computational**

This project is in the area of photonic organic materials for energy applications. When an electron is transferred to an excited state on photon absorption by an organic molecule, its chemical bond strengths may change. This can result in significant changes to the equilibrium molecular structure. When a photon is absorbed in a vertical transition, the molecule may be in an electronically and vibrationally excited state. If the molecule has time to relax to its new equilibrium structure within the exited state lifetime and then emits a photon (fluorescence), the emitted photon may have significantly longer wavelength than the absorbed photon. This shift in wavelength is known as [Stokes shift](#) after its discoverer, the renowned Irish physicist, G. G. Stokes. In simulating organic light emitters, it is therefore essential to be able to determine the structures of molecules in their excited states. This project will afford the opportunity to use time-dependent density functional theory codes to study the light absorption and emission properties of a series of organic molecules with applications as organic LEDs, especially the change in molecular equilibrium geometry in the excited state.

[38] Simulation of Stokes shifts in light emission by organic materials

**Supervisor:** Prof. Charles Patterson
**Contact Prof. Patterson**

**Computational**

Some optical excitations in matter result in transfer of an electron between two distinct parts of a molecule or from one molecule to a neighbouring molecule. These are known as charge transfer (CT) excitations. When a CT excitation occurs between two molecules there is a coulombic attraction between the negatively charged acceptor molecule and the positively charged donor molecule. The donor and acceptor molecules are unbound in the ground state but become bound in the excited state. This is known as an exciplex. Exciplexes are finding applications as light emitters for organic LEDs (OLEDs) because of this delocalised nature of the excited state. Optical excitations exist as spin-parallel or anti-parallel excited states called triplets and singlets. When excited states are formed by optical pumping (or by injecting electrons and holes as in an OLED) there are three triplet excited states formed for every singlet. However, only the singlet states fluoresce readily (photon emission). Exciplexes are important for OLED emitters as the delocalised nature of the CT excited state means that singlet and triplet excited states have similar energies. This allows thermal interconversion of triplets to singlets and an increase in the theoretical efficiency from 25% to 100%. This project will use many-body quantum methods to calculate properties of exciplexes.

[39] Many-body theory of exciplexes for OLED devices

**Supervisor:** Prof. Charles Patterson
**Contact Prof. Patterson**

**Computational**

Molecular dynamics is a technique for simulating the atomic structure of matter at relatively low computational cost. In this project you will learn to use the LAMMPS code to simulate structures of organic light emitters embedded in a host matrix. The object will be to generate an ensemble of structure snapshots for use in excited state calculations, either as finite aggregates or as periodic systems. Organic LEDs with high quantum efficiencies generally consist of host materials with higher singlet and triplet and excited energy levels than the thermally activated delayed fluorescence TADF-OLED emitter in order to channel excitation energy into the emitter. In particular we are interested in how the emitter packs in the host, whether there are emitter-host interactions which may affect charge transfer rates or emission frequencies.
Electron scattering from spin-orbit enhanced quantum dots in graphene

Supervisor: Dr. Stephen Power

Contact Prof. Power

Computational
Can be done remotely

Graphene has an unusual electronic dispersion relation that bears closer resemblance to that of light than to that of a conventional semiconductor. In fact, many features of graphene are well-described using the relativistic Dirac equation from quantum electrodynamics in place of the more standard Schrödinger equation.

Very recent research proposes using other materials to induce features such as spin-orbit coupling (SOC -- which is naturally weak in graphene) in graphene whilst maintaining the excellent electronic transport that makes it so appealing for applications. This would allow a higher degree of control over the "spin" degree of freedom than is currently possible.

This project will study the analytics of electron scattering from regions of enhanced SOC in graphene in order to determine the characteristics of materials that give the greatest degree of control of spin behaviour. The student will:

- Learn the tight-binding and Dirac spinor representations of electrons in graphene
- Examine how barrier and spherically-symmetric scattering geometries can be solved using the Dirac approach for simple potential terms
- Investigate the different Hamiltonians required to describe proximity-induced spin-orbit coupling in graphene, and how these are written in Dirac notation
- Solve the full scattering problem for a range of realistic parameters, and calculate the spin-filtering and spin-splitting efficiencies of these systems.
Electronic states in defected fractal lattices

Supervisor: Dr. Stephen Power

Contact Prof. Power

Computational
Can be done remotely

Recent experimental advances allow for geometric electronic fractals to be created and characterised. In these systems, electrons are confined to a self-similar fractal geometry with a dimension between one and two. Controlling the positions of molecules on metallic surfaces allows for precise, large-scale artificial atomic lattices to be investigated using scanning tunneling microscopy and spectroscopy.

This project will explore the electronic properties of such systems using computational methods. The goal is to understand how additional designer behaviours can be introduced by impurity engineering. We will consider the roles that vacancies, anisotropy (strain) and external fields can play in tuning the lattice properties.

The student will:

- Learn the tight-binding representation of electrons in pristine lattices;
- Implement recursive Green’s function methods to calculate electronic properties of larger structures;
- Calculate how the properties of the system change as vacancies are introduced or as strain breaks the symmetry of the structure;
- Introduce an external magnetic field and investigate quantum Hall behaviour in the system;
- Generalise to higher dimensions (Sierpinski tetrahedra)

Transparent conducting oxides (TCOs) are a material class which exhibit the unique benefit of being both optically transparent and electronically conductive, properties which are often found to be in direct opposition to one another. However, the majority of currently applied TCOs are formed from expensive and rare elements, such as indium. As a result, there is a drive to reduce costs and increase sustainability in the industry. One promising material which can act as a solution to this ongoing problem is amorphous Zinc Tin Oxide (a-ZTO). a-ZTO has the benefit of being formed from common elements, having excellent electrical and optical properties and a non-crystalline (amorphous) structure. This lack of crystal structure drastically reduces the difficulty in forming it and gives it a resistance to damage due to bending, making it also potentially useful in flexible electronics. One of the most popular low-cost methods of depositing a-ZTO is spray pyrolysis. In this method a set of Zinc and tin containing materials are dissolved in a liquid and sprayed onto a heated substrate where the compound forms. The formation processes that occur at the substrate are complex and dependent on a wide range of parameters (tin and zinc source, transparent liquid, gas atmosphere temperature etc.) which can have distinct effects on the finished films. As a result, understanding the influence of the different deposition parameters used can be complex. In this project the researcher will use optical analysis techniques to examine the morphology and optical structure of spray deposited Zinc Tin Oxide, focusing on how the choice of deposition conditions can influence the properties of the resulting film, with particular attention paid to the nature of the starting choice of zinc and tin source materials. To do this the researcher will start by making use of both UV-Vis spectrophotometry, for transmission, reflection and light scattering measurements. However, the bulk of the project will involve optical fitting using data obtained from Ellipsometry, a much more detailed optical measurement system that determines the underlying dielectric function of the material. In doing so the researcher will determine how the refractive index, optical absorption, surface structure bandgap and density is influenced via choice of deposition parameters. In doing so the researcher will gain an insight into the different processes that take part in forming the material during deposition.
Quasi-classical spin dynamics in compensated ferrimagnetic systems: a 1D/2D approach to understanding pinning and nucleation of domain walls and skyrmions

**Supervisor:** Prof. Plamen Stamenov

The project will involve the theoretical and computational modelling of spin dynamics in a relatively new class of magnetic materials—the Zero-Moment Half-Metals (ZMHM). ZMHMs are posing a challenge to understand and exploit a rather unique for spin electronics combination of high bulk spin polarisation, stray field immunity and intrinsically high resonance and switching frequencies, effectively limited by the exchange energy in the system. Nano-scale ultrafast and non-volatile MRAM elements and terahertz oscillators are only two examples of applications, which could benefit hugely from the utilisation of ZMHMs. The complete theoretical (ab initio) modelling of these materials is rather challenging, for the incomplete knowledge of their intrinsic and extrinsic disorder and the fine details of the effective interactions in the system, including higher order exchange and spin-orbit torques. Here a divide and conquer approach will be used to theoretically and computationally model within an effective spin Hamiltonian approach the dynamics of domain walls and other topological objects, such as skyrmions, which become possible with the inclusion of Dzyaloshinskii-Moriya interactions. The influence of magnetic field, electric current and local pinning on the mobility and dissipation within these objects will be clarified. The work will start with an existing 1D code for quasi-classical spin simulation and transition it into a 2D version towards the end of the project, looking for phenomena that cannot be mapped-down successfully in 1D.

Optically-Excited Magnetometry of Spin-Crossover Compounds

**Supervisor:** Prof. Plamen Stamenov

The project will involve the experimental characterisation of already synthesized metal-organic spin-crossover compounds (in collaboration with the group of Prof. Wolfgang Schmitt, TCD, Chemistry) using SQUID magnetometry, at low temperature, while exciting the molecules in a spectrally selective fashion. Selected compounds, which have already been shown to exhibit low-spin/high-spin transitions at a convenient temperature region (below room temperature) will be subjected to monochromated and modulated near-infrared, visible and near-ultraviolet light, while their magnetic moment is measured, within the variable temperature environment of a commercial SQUID magnetometer (MPMS XL, Quantum Design, CA), capable of providing magnetic fields of up to 5 T. The influence of the photon excitation on the magnitude and temperature of the spin-transitions in these compounds will be studied, together with any low-frequency quantum-mechanical state population dynamics (with a dynamic range of up to 20 kHz). The final year project student will receive training in high-end SQUID magnetometry and will be directly involved in the construction and testing of the light delivery system and the actual sample measurements and analysis. No spectrally-dispersive, or dynamic measurements of this type have been reported to date. A successful study would be expected to yield a plethora of information about the energetics and dynamics of the spin-transitions in metal-organic molecular compounds, and establish framework of data acquisition hardware and software, and the data fitting models to complement that. The detailed understanding of the spin states in metal-
organic complexes is key to their down-selection and eventual deployment as molecular q-bits or memory cells in the area of quantum computing.


Supervisor: Prof. Plamen Stamenov

Experimental

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$_x$Ga, in a thin film form. ZMHMs have the potential to offer the rather unique for spin electronics combination of high bulk spin polarisation, stray field immunity and intrinsically high resonance and switching frequencies. Nano-scale memory elements and terahertz oscillators are only two 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 determine the anisotropy of the conductivity and Hall effect tensor in these, typically tetragonally-distorted ZMHMs. The measurements 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. Fitting models and visualization software will be prepared, taking into account the magnetic space-group and general symmetries of the crystalline films, which will allow for the quantitative interpretation of the anisotropy and correspondingly the strength of the various spin-orbit and exchange interactions in the system. The information gained will be critical for the development of prototype magnetic devices working in the high-GHz and low-THz regions.

[47] High-Power Narrow (K and Ka)-Band Waveguide-based Ferromagnetic Resonance in Thin Magnetic Films and Microstructures: Simultaneous inductive and SQUID-based Detection

Supervisor: Prof. Plamen Stamenov

FerroMagnetic Resonance (FMR) has been instrumental in characterising the magnetisation and the effective anisotropy fields in a large number of bulk materials and some repetitive microstructures. Conventional FMR relies on narrow band inductive excitation and detection of the precessional motion of the local magnetisation averaged over some volume typically of the order of mm$^3$. The superb sensitivity of modern SQUID-based magnetometers allows for a different approach towards the FMR measurement problem direct measurement of the precession cone angle as a function of frequency, applied magnetic field and temperature, by detecting the mz component of the magnetisation and the small decrease in its value upon microwave excitation mz. Previously, we have demonstrated the capabilities of this new technique, using broadband strip lines as waveguides. These, however become inefficient at frequencies beyond 20 GHz. The project will involve the preparation of a waveguide structure for the transmission of high-frequency microwaves (18 to 40 GHz) into the sample environment of a commercial SQUID magnetometer and the measurements of FMR by both SQUID-based and conventional inductive techniques. Within this study, a source, waveguide and sample insert will be constructed and tested, augmenting the frequency capability of the existing broadband system (0.5 to 20 GHz) shown on the figure below. A success in this endeavour will enable the study of an exciting new
range of half-metallic low-moment ferromagnetic materials with very high resonance frequencies, which will support microwave magnetics in the future 5G network deployments and beyond.

[48] Sub-picosecond pulsed induced demagnetisation of magnetic materials:
resolving the role of the exchange interaction

Supervisor: Prof. Plamen Stamenov
Contact Prof. Stamenov
Experimental

The irradiation of a magnetic material by a femtosecond light pulse can trigger a subpicosecond loss of magnetic order. The mechanisms behind this ultrafast demagnetisation have been widely studied in ferromagnets. In ferrimagnets, where two magnetic sub-lattices are antiferromagnetically coupled, it is assumed that an additional ultrafast demagnetisation driven by the inter-sublattice magnetic exchange could occur. Such angular momentum conserving demagnetisation could theoretically drive a faster demagnetisation on the 100 fs timescale. Concomitantly, we recently discovered that a femtosecond light pulse is sufficient to control the magnetisation of the compensated ferrimagnet Mn$_2$Ru$_x$Ga and believe that the ultrafast demagnetisation via the exchange interaction is a determining factor to explain the single pulse all-optical switching in this material.

In this project, we will elucidate the timescale of a thermal pulsed-induced demagnetisation purely driven by inter-sublattice exchange of magnetic moment, deduce requirements to achieve exchange driven sub-picosecond magnetic switching and shed light on the fingerprint of such switching. The student will learn to use the atomistic simulation software Vampire to simulate: (1) static magnetization versus temperature behavior based on experimental data and (2) the dynamics of the exchange of magnetic moment between sublattices following various initial conditions. This work will help to establish working hypothesis for future experiments.
Machine learning density functional theory at finite temperature

Supervisors: Dr. Rajarshi Tiwari and Prof. Stefano Sanvito

Computational
Can be done remotely

Machine learning density functional theory at finite temperature
Density functional theory (DFT) consists in a strategy to solve the many-electron problem alternative to simply solving the Schrödinger equation. It is based on the Hohenberg-Kohn theorem (1), which establishes that the ground state energy of a system is a universal functional of the electron density. This functional is minimised at the ground-state density, where it returns the ground-state energy. The same theory can be applied to lattice models such as the Hubbard model, where now the electron density is replaced by the site occupation (2). Unfortunately the functional is not known, so that one needs to approximate it. Recently an alternative strategy became possible, namely that of constructing numerically exact functionals by using machine learning methods (3). In this case one first solves the problem exactly for simple systems and then uses such data to interpolate a functional. Neural networks appear particularly suitable to perform such task. In this project we will attempt to use the same procedure, but this time for finite temperature (DFT). In this case the system energy is replaced by the Helmholtz free energy and the ground-state density by the equilibrium one. In particular we will construct a numerical finite-temperature energy functional for the spinless Hubbard model.

During the project the student:
1. Will familiarise with many-body problems and with DFT
2. Will learn the basics of machine learning
3. Will construct a neural network describing the finite-temperature energy functional

Requisites: Familiarity with python
(1) P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964)

Machine-learning force fields for the phase diagram of oxides

Supervisors: Dr. Allessandro Lunghi and Prof. Stefano Sanvito

Computational

Machine-learning force fields for the phase diagram of oxides
Machine learning is rapidly becoming a powerful tool to discover patterns in apparently unrelated data (1). It comprises a range of computational methods, which underpin the most diverse applications, going from image recognition to natural language processing, to complex optimisation and classification problems. The use of machine learning in materials science instead is in its infancy (2), mostly because of the relatively poor availability of data. This issue is, however, mitigated by the access to large databases of computed properties, so that machine learning algorithms can serve the purpose of replacing numerically costly computational methods. One particular use of machine learning in materials science is related to the construction of highly accurate atomic potentials. These can describe the interaction between atoms at a level of accuracy comparable to that of the much more demanding first principles methods at a fraction of their computational cost.
this project we will explore how such machine-learning force fields can predict the phase diagram of binary compounds. In particular we will study how the force fields can describe the phase diagrams of binary transition-metal oxides, where the valence of the metal may vary across the phase diagram. Particular attention will be dedicated to error analysis and to the understanding on how the predictions can be trusted for unknown compounds.

The students will:
1. Learn the basics of machine learning
2. Construct a machine-learning force field for a binary phase diagram
3. Extract elementary properties with the machine learning force field

Requisites: Familiarity with python
(1) T. Hastie, R. Tibshirani and J. Friedman, The elements of statistical learning, Springer.


Supervisors: Dr. Rajarshi Tiwari and Prof. Stefano Sanvito
[Contact Dr. Tiwari]

Computational
Can be done remotely

Density functional theory (DFT) offers an alternative way to tackle the many-body problem. The idea is that the ground-state energy of a system can be found by minimizing a universal energy functional of the electron density (1). Such functional exists but its explicit exact form is unknown, so that it needs to be approximated. Recently an alternative strategy became possible, namely that of constructing numerically exact functionals by using machine learning methods (2). In this case one first solves the problem exactly for simple systems and then uses such data to interpolate a functional. Neural networks appear particularly suitable to perform such task. In this project we will attempt to use the machine-learning strategy to learn the functional that solves a model involving both electronic and vibrational degrees of freedom. This is the Hubbard-Holstein model (3), which is often used to describe phases of matter where the interaction with vibrations determine the ground-state properties of the system (e.g. superconductivity, polaronic distortions, etc.). Here the task will be that of constructing a functional where both the electron density and the vibrations density are taken into account, in the same spirit of density functional theory for superconductivity (4).

Throughout the project the student:
1. Will familiarise with many-body problems and with DFT
2. Will solve exactly the Holstein model for simple systems
3. Will learn the basics of machine learning
4. Will construct a neural network describing the finite-temperature energy functional

Requisites: Familiarity with python
(1) P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964)
Machine learning methods (1) are rapidly becoming an alternative to complex electronic structure theories in the description of molecules and solids. In general, machine learning schemes find pattern in data. In the case of quantum chemistry and materials science, one of the tasks is to correlate the geometry of a molecule (the position of its atoms) to its properties (2). This is not an easy task, since the molecule representation needs to be compatible with machine learning. In general, a molecule is described by a vector (e.g., a vector with the coordinates of the atoms). One has then to ensure that two identical vectors correspond to two identical molecules, that similar vectors correspond to similar molecules, that identical molecules located in different places are described by the same vector, etc. This means that the decision on how to represent a molecule is crucial to determine whether a machine-learning strategy can be used at all. In this project, we will explore how different molecule representations perform in predicting the molecule properties. In particular, we will consider various versions of multipolar expansion and how these can be used to compute the molecule total energy. To simplify the problem, all molecules will be described by a simple pairwise potential, such as the Lennard-Jones one.

Throughout the project, the student:
1. Will familiarise with machine learning methods
2. Will construct a pairwise potential to generate the molecule data
3. Will construct a machine learning representation of the molecules
4. Will construct a neural network to describe the molecules energy

Requisites: Familiarity with python

(1) T. Hastie, R. Tibshirani and J. Friedman, The elements of statistical learning, Springer.
ZnO nanostructure is one of the most-intensively-investigated materials in recent years because of its extraordinary properties and remarkable potential applications. This project aims to understand the tuning the photoemission of ZnO nanostructures via focused-ion beam irradiation. The He$^+$ beam induced surface sputtering, lattice damage and strain field will adjust the dimensions, surface roughness, and refractive index of the ZnO sample. This changes the Whispering Gallery Mode (WGM) in the ZnO nanostructure. We will develop a COMSOL model and simulate the light emission of ZnO nanostructures to identify the factors that are responsible for the luminescence tuning.
Ground and space measurements of light pollution - closing the gap

**Supervisor:** Prof. Brian Espey

**Contact Prof. Espey**

**Computational**

**Can be done remotely**

Historical and current night sky light measurements taken from the ground (including from TCD) will be compared with satellite observation of light sources. The goal of this work is to estimate the amount of light scattered by molecules and aerosols and to determine whether there has been any growth in light waste, particularly since the introduction of cheaper, and now ubiquitous, LED lighting. Using these data an attempt will also be made to estimate the region around a ground site that predominantly contributes to the local sky pollution levels. This project will involve the use of the R shareware package, which can be run on a laptop. For information on the software see [here](#).

City light output in the time of COVID-19

**Supervisor:** Prof. Brian Espey

**Contact Prof. Espey**

**Computational**

**Can be done remotely**

The COVID-19 outbreak provides us with an unprecedented opportunity to study how the reduction in manufacturing and commercial activity during the worldwide COVID-19 lockdown impacts on air pollution and light output. The project will use night-time imaging from the International Space Station and NASAs VIIRS satellite together with air pollution and imagery data from ESAs Copernicus satellite to study the effect of a reduction in economic output on light pollution. This project will involve the use of the R shareware package, which can be run on a laptop. Information on the software is available [here](#).

High Speed Monitoring of Solar Radio Bursts

**Supervisor:** Prof. Peter Gallagher, DIAS, Fitzwilliam Place and Dunsink Observatory

**Contact Prof. Gallagher**

**Computational**

**Can be done remotely**

Low frequency radio waves at < 100 MHz can offer an insight into the properties of plasmas processes that occur during energy release in the solar atmosphere, such as flares and coronal mass ejections. Modern low frequency radio telescopes, such as the Low Frequency Array (LOFAR; www.lofar.org), have been developed using a large number of low cost antennae together with receiver systems that use recent advances in digital signal processing. In this project, the student will set up and observe the Sun at 10-90 MHz using a low frequency antennae connected up to an FPGA-based signal processing unit. The student will compare the performance of this system with coordinated observations from antennas at the [Irish Low Frequency Array](#) in Birr Castle. Note: This project would best suit a student with an aptitude for instrumentation and software development.
Atmospheres of alien worlds: exploring transmission spectra of exoplanets using machine-learning techniques

**Supervisor:** Prof. Neale Gibson

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 a technique called transmission spectroscopy. This 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. This project will use data from the Hubble Space Telescope, or simulated data, to test advanced statistical techniques to model the impact of time-dependent instrumental systematics on the analysis of transit light curves, aiming to recover atomic and molecular features in planetary atmospheres using low-resolution transmission spectroscopy from space-based observations.

Atmospheres of alien worlds: searching for new atmospheric species via high-resolution transmission spectra

**Supervisor:** Prof. Neale Gibson

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 a technique called transmission spectroscopy. This 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. This project will use a technique called Doppler-resolved transit 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 emphasis will be on developing atmospheric models of planetary atmospheres and searching for atomic, ionic and molecular species in ultra-hot Jupiters.
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 a technique called transmission spectroscopy. This 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. This project will use a technique called Doppler-resolved transit 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 emphasis will be on exploring new machine-learning and/or statistical tools to recover information on the planet’s atmosphere.
[60] Stars that directly collapse to black holes

**Supervisor:** Prof. Jose Groh  
**Contact Prof. Groh**  
**Computational**  
**Can be done remotely**

While the vast majority of massive stars are expected to explode as bright supernovae, about 10% of massive stars are expected to die gently without producing supernovae. These stellar deaths do not produce a bright explosion, and the star directly collapses to form a black hole. In this project, the student will investigate the mass range of stars that could produce direct-collapse black holes and predict the final mass of the black hole. This will be achieved by computing state-of-the-art numerical stellar evolution models, which will allow the student to predict the brightness of stars just before death. The results of this project will shed light on the different types of stellar deaths and their progenitors.

[61] The properties of the first stars in the Universe

**Supervisor:** Prof. Jose Groh  
**Contact Prof. Groh**  
**Computational**  
**Can be done remotely**

The Universe was a relatively quiet place for about 400 millions years after the Big Bang. From that point on, the formation of the first stars drove dramatic changes in the Universe, with the synthesis of new chemical elements and emission of large amounts of energetic photons. There are significant efforts to observe the signatures of the first stars, but no direct detection has yet been made. The goal of this project is to investigate the properties of the first stars in the Universe using modern stellar evolution models. For doing that, the student will compute novel state-of-the-art numerical models developed by my group. The predictions regarding the first stars will be important for interpreting future observations that will become available when the James Webb space telescope is launched.

[62] Effects of stellar populations in the nearby Universe

**Supervisor:** Prof. Jose Groh  
**Contact Prof. Groh**  
**Computational**  
**Can be done remotely**

Massive stars evolve on timescales of just a few million years. Due to their rapid evolution and the physics of star formation, they are easily outnumbered by their low-mass siblings. Albeit rare, massive stars are essential constituents of a stellar population, being the main contributors to the input of ionizing photons, energy, and momentum into the interstellar medium and playing a key role in the chemical enrichment of their host galaxy. In this project, the student will employ the latest generation of stellar evolution and radiative transfer models to obtain the properties of stellar populations found in the nearby Universe, for a range of initial masses and ages. This will allow the prediction of how integrated stellar populations evolve, in particular their spectroscopic signatures.
How does explosive magnetic reconnection in Saturn’s magnetosphere drive intense radio emissions?

**Supervisor:** Prof. Caitriona Jackman, DIAS, Fitzwilliam Place

**Contact Prof. Jackman**

**Computational**

**Can be done remotely**

NASAs Cassini mission to Saturn was one of the most ambitious interplanetary spacecraft ever built. It spent a total of 20 years in space, and successfully orbited the planet Saturn from 2004 to 2017. This project will focus on analysis of data from the Cassini spacecraft, including from the magnetometer instrument sampling Saturn’s magnetic field, and the radio and plasma wave science instrument measuring powerful radio emission from Saturn’s polar regions. The aim is to quantify the link between explosive magnetic reconnection events identified from signatures in the magnetometer data and intense, low frequency radio emissions from Saturn’s auroral regions. Data from orbital spacecraft like Cassini can provide direct evidence of energetic processes like magnetic reconnection, and help us to learn about the fundamental physics behind these explosive phenomena. In order to make the link between magnetic and radio signatures, the student will draw on catalogues of events which emerge from application of machine learning algorithms, providing exposure to this growing area of data-intensive science. This is an observational project that requires Python for data analysis.

Radio emission from nebulae around massive stars

**Supervisor:** Prof. Jonathan Mackey, DIAS, Fitzwilliam Place and Dunsink Observatory

**Contact Prof. Mackey**

**Computational**

**Can be done remotely**

Ionized plasmas emit radiation at radio wavelengths via two main mechanisms: Bremsstrahlung (“braking radiation”) from thermal electrons with kinetic energy around 1 electron-volt (1 eV \( \sim 10^{-19} \) Joules), and synchrotron radiation from relativistic electrons with energies from mega-electron-volts (MeV) up to tera-electron-volts (TeV). Nebulae around massive stars emit through both of these processes. We use both radio observations and fluid-dynamics simulations of nebulae around massive stars to investigate their efficiency in accelerating electrons and protons to TeV energies. For this project the student will learn about radiation mechanisms for interstellar plasmas, computer simulation of fluid dynamics, and some basics of analysing radio astronomy data from LOFAR and the VLA. The aim is to compare simulations with observations, developing criteria that can determine whether a computer model is a good representation of a given nebula. Programming will be mainly with Python and some C++ programming. The student will use Calculus and Linear Algebra to develop discrete representations of the equations describing Bremsstrahlung and Synchrotron emission, that can be used to generate emission maps from simulations.
Spectroscopic modelling of thermonuclear supernovae

Supervisors: Dr. Mark Magee and Prof. Kate Maguire

Contact Dr. Magee

Computational
Can be done remotely

Supernovae are some of the most explosive events in the universe. They can enrich the cosmos with synthesised heavy elements and can outshine entire galaxies for a short period of time. Type Ia supernovae are the most commonly observed supernova type, and are fundamental to cosmology and our understanding of the Universe. In spite of this, their exact origin remains unclear. By taking spectra of these supernovae we are able to interrogate whether suggested explosion scenarios are in agreement with what is observed. This project is focused on constructing models from proposed explosion scenarios and comparing these to observations. Some basic background in programming (Python) would be beneficial, but is not essential.

Unveiling the explosion geometries of massive-star supernovae

Supervisor: Dr. Simon Prentice and Prof. Kate Maguire

Contact Dr. Prentice

Computational
Can be done remotely

Type Ib and Ic supernovae are the resulting explosion of massive stars stripped of their hydrogen envelope. In the nebular phase these transients emit a significant amount of flux through a forbidden oxygen line. As oxygen forms the majority of the ejected material this line is a useful diagnostic for ejecta mass and asphericity. In this project the student will collate nebular spectra of SNe Ib/c and characterise the shape of the oxygen emission line profile. They will then look for correlations with known properties of these objects obtained from the literature to see if late-time asphericity is also evidenced in the early-time observables. This project will involve some coding in Python.

Type Ia supernovae: Cosmology and their explosion properties

Supervisor: Prof. Kate Maguire

Contact Prof. Maguire

Computational
Can be done remotely

Supernovae are the extremely luminous explosions of stars at the end of their lives. The use of a particular type of exploding star, Type Ia supernovae, as probes of cosmology is now well established but how exactly they explode is still not well understood with multiple competing scenarios for producing Type Ia supernova explosions. One way of potentially distinguishing between these scenarios is by constraining the diversity in their optical spectra and light curves very soon after explosion. This has only become possible with new state-of-the-art transient surveys such as the Zwicky Transient Factory (ZTF) that are scanning the sky looking for new events multiple times a night. The aim of this project is to use day zero ZTF data to connect spectral signatures of key elements in the outer layers of the supernovae (e.g. carbon, oxygen, calcium) to their explosion channels. This will allow improved cosmology samples to be selected.
and also to quantify the impact of spectral and light curve diversity on Type Ia supernova cosmological analyses.

[68] Statistics of Solar Eruptions

Supervisor: Dr. Sophie Murray
Contact Dr. Murray
Computational
Can be done remotely

Space weather describes the dynamic conditions in Earth’s outer space environment. Space weather forecasting has developed rapidly in recent years, with the threat of a severe space weather event increasing in importance as society becomes ever more dependent on technology. These severe events originate from solar eruptions (solar flares, coronal mass ejections, and solar energetic particle events) and solar activity is now closely monitored by operational forecasting centres worldwide to provide sufficient warning of solar eruptions that may impact us here on Earth. However it is still not clearly understood why, when, and how these eruptions may occur. This project will involve statistical analysis of several solar eruption event catalogues from over twenty years of satellite observations of the Sun. Analysis will be undertaken using the Python programming language to link and compare different types of eruptive events. The results will provide insight into what eruption characteristics are associated with extreme events, which will ultimately aid future efforts to improve the accuracy of space weather forecasts.

[69] Leaky atmospheres in exoplanets: the strength of H-alpha transits

Supervisor: Prof. Aline Vidotto
Contact Prof. Vidotto
Computational
Can be done remotely

Atmospheric escape plays a key role in planetary evolution, planetary population, and habitability. Because of the close proximity to their host stars, close-in exoplanets receive an intense flux of high-energy stellar irradiation. This irradiation heats planetary atmospheres, causing them to inflate and more likely to outflow through a hydrodynamic escape mechanism. Evaporation can be seen during spectroscopic transits and, in particular, the hydrogen-dominated atmospheres of gas giants have been observed in Ly-alpha (n=2 to n=1 transition in the UV) using Hubble. Given that space observations are very expensive, several works have attempted to detect escaping hydrogen in the H-alpha line (n=3 to n=2 transition in the visible), which can be conducted from ground-based telescopes. Surprisingly, in spite of the huge absorption in Ly-alpha, only a few gas giants show significant absorption in H-alpha. The aim of this project is to investigate why this happens. For that, the student will model atmospheric escape of close-in exoplanets using hydrodynamic simulations and compute transit observations in H-alpha and Ly-alpha.
The role of the tachocline in stellar magnetic field generation

Supervisors: Dr. Gopal Hazra and Prof. Aline Vidotto

The shear layer between the radiative zone and convective zone is known as the tachocline. The tachocline plays an important role in magnetic field generation in the sun-like stars. Given that low-mass stars are fully convective, they do not present a tachocline and thus, it has been predicted that their magnetic fields do not behave like those in solar-like stars. However, recent observations have shown that fully convective stars show similar magnetic activity behaviour as sun-like stars, leading us to question whether the tachocline is really important for magnetic field generation. In this project, the student will investigate the role of the tachocline in stellar magnetic activity by modelling magnetic field generation in stars with and without the tachocline. The student will learn to use existing codes in 2D. This is a theoretical project and requires use of Python or IDL.

Modelling the propagation of cosmic rays in protoplanetary disks observed with ALMA

Supervisors: Dr. Donna Rodgers-Lee and Prof. Aline Vidotto

Disks of dust and gas surround young stars and are the birthplace of exoplanets. How these protoplanetary disks physically and chemically evolve to form pre-biotic molecules depends sensitively on disk ionisation. X-rays from the central star and radioactive decay alone cannot sufficiently ionise disks to explain certain observations. Stellar energetic particles, known as cosmic rays, may play an important role in disk ionisation. This project focuses on constraining the contribution that stellar cosmic rays have to the overall ionisation rate in protoplanetary disks. Specifically, the student will apply a cosmic ray propagation code to exciting recent ALMA observations and will derive the transport properties of cosmic rays that best fit the observational data. This is a computational project that will use existing codes in python and requires basic programming skills.