Title: A new approach to solar harvesting using a nanoscale rectenna system

Supervisor: Associate Professor Dominic Zerulla (dominic.zerulla@ucd.ie)

One of the most important challenges globally is to provide energy from renewable sources to stop the emission of greenhouse gases entering the atmosphere. The importance of which cannot be overstated as is evidenced by the current projections for global warming. The only regenerative source which can satisfy the global energy demands now and in the foreseeable future is the sun.

This project has the ability to completely innovate the current solar energy harvesting technology as it moves away from traditional concepts by using a new paradigm from which to generate energy by using carbon nanotubes as antennas at the nanoscale.

The core of the here proposed research is to optimize the integration of these carbon nanotubes into an a-symmetrical quantum mechanical environment. The interface between the two needs to have rectifying properties on very small spatial scales hence providing a novel way of generating energy from sunlight. This concept has the ability to break the Shockley-Queisser limit of 32% energy efficacy and is predicted to be capable of having a theoretical efficiency of 44% thus having the capacity to revolutionize energy generation.

Advanced wavefront sensing and control for optical microscopy

Supervisor: Dr. Brian Vohnsen (brian.vohnsen@ucd.ie)

Accurate sensing and control of aberrations is vital in many fields including astronomy, microscopy, ophthalmology and laser-based light sources. With this project we wish to explore wavefront sensing and control for advanced optical microscopy. A Hartmann-Shack wavefront sensor is commonly used in adaptive optics systems but blind deconvolution methods offer significant advantages by avoiding the use of a camera and allowing for single-pixel-based imaging. Optical control of aberrations can also be used to image through opaque highly scattering optical materials, to modify the point-spread-function in optical imaging, and for beam engineering. We will use the knowledge gained to develop novel wavefront sensors as viable alternatives to the Hartmann-Shack wavefront sensor and spatial light modulators to control polarization and exposure conditions of biologically relevant samples. This includes imaging of ocular tissues with two-photon microscopy in collaboration with US-based collaborators and novel material pattering techniques for waveguide-based ophthalmic materials. Systems and applications will be optimized in terms of resolution, contrast and sensitivity.

Advanced Optical Imaging Group, School of Physics, University College Dublin, Ireland

Title: Black holes and exploding stars

Supervisor: Dr Morgan Fraser (morgan.fraser@ucd.ie)

Every night, survey telescopes scan the sky looking for exotic astronomical transients such as supernovae, stellar eruptions, and flares from accreting black holes. Recently, we have had considerable success finding a rare class of transients called "tidal disruption events" (TDEs), which occur when a star passes within the tidal radius of a massive black hole, and is ripped apart (Leloudas, Fraser et al, 2017, Nature Astronomy). Such TDEs are accompanied by a burst of light across the electromagnetic spectrum, and can be used to probe otherwise unobservable black holes. As part of this PhD, you will use world class telescopes (including the European Southern Observatory in Chile) to find, characterise and understand TDEs. Using observational data, and in collaboration with theoreticians, you will work to unlock some of the most mysterious objects in the Universe.

Title: Central Exclusive Physics at LHCB

Supervisor: Prof Ronan McNulty (ronan.mcnulty@ucd.ie)

The strong force is mediated by coloured gluons so interactions at the LHC usually produce hundreds of hadrons. However, colourless propagators (e.g. Pomerons) also exist in QCD and interactions via two Pomerons result in a very unusual experimental signature at the LHC of just a very few particles (Central Exclusive Production). Studying these tells us about the fundamental nature of QCD, allows a determination of the gluon content of the proton, and is a mechanism to discover exotic particles like tetraquarks and glueballs.

In this Ph.D. project the student will go to CERN, collect data on the LHCb experiment and analyse it to obtain a sample of Central Exclusive Events. Signals for known resonances (Jpsi, rho, f2) will be found and their cross-sections determined. Then searches will be made for unknown resonances whose observation would be evidence for new tetraquark states, glueballs, or new physics.

Further reading:

arXiv:1409.8113, arXiv:1407.5973, arXiv:1401.3288)

Title: Detecting gamma-ray bursts using CubeSats in the gravitational waves era

Supervisor: Sheila McBreen (sheila.mcbreen@ucd.ie)

Abstract: Gravitational waves (GW) were detected for the first time in 2015 thereby opening up an uncharted realm of astrophysics. GWs from a neutron star merger in coincidence with a short gamma-ray burst in a nearby galaxy were detected August 2017 marking first discovery of a electromagnetic counterpart of a gravitational wave source. There is an urgent need for gamma-ray space missions during the GW era and this need can be met by a coordinated fleet of small satellites. CubeSats are miniaturised platforms that carry payloads from 1-12 U (where 1 U = 10 cm^3 and are delivered into orbit with other satellites, substantially reducing the cost and development lifecycle. The Gamma-ray Investigation of the Full Transient Sky (GIFTS) project will further develop a novel gamma-ray module previously developed in UCD and for the EIRSAT-1 mission which can be replicated and used in a constellation of gamma-ray small satellites. The GIFTS CubeSat module design will comprise scintillators, Silicon PhotoMultipliers plus digital readout and be designed for a 6 U CubeSat. GIFTS will collaborate with colleagues at NASA, ESA, NSSTC and UNH, SensL and IDEAS.

Title: Fundamental physics and new messengers

Supervisor: Professor Lorraine Hanlon (lorraine.hanlon@ucd.ie)

Future gamma-ray space observatories will operate in a maturing gravitational wave and multi-messenger epoch. The recent detection of a gamma-ray burst and a gravitational wave event associated with the merger of two neutron stars confirms the fundamental physics that can be revealed by such events. New constraints on, for example, the deviation of the speed of gravity from the speed of light and on violations of Lorentz invariance and the equivalence principle, have been made possible by this landmark discovery. To prepare for this new era of astrophysics, quantitative assessment and optimisation of the performance of future gamma-ray experiment designs will be carried out, using computer simulations and laboratory measurements, in collaboration with global partners and space agencies.

Title: Fundamental theory for novel nanoelectronic devices

Supervisor: Dr Andrew Mitchell (andrew.mitchell@ucd.ie)

When nanoscale components are incorporated into electronic circuits, the laws of quantum mechanics govern their basic properties. Striking phenomena such as entanglement and quantum interference can appear, and have no classical analogue. The next generation of miniaturized electronics must overcome the limitations of traditional design paradigms by exploiting the novel functionality of the nano. However, the fundamental physics of nanoelectronic devices is notoriously complex and in many cases a theoretical framework to understand their physical properties is missing. Presently the experimental approach is ad hoc and device characterization is poor. Clearly basic theoretical research in this area is a prerequisite for future rational design of new devices with novel quantum functionality.

A Thomas Preston Scholarship would allow a talented student to undertake important cutting-edge work in this emerging area of theoretical nanoscience. In particular, the focus will be on the underlying theory of single-molecule transistors, where new possibilities arise from the complex interplay between quantum interference due to competing electron transport pathways through the molecule, and entanglement from strong interactions between the highly confined electrons. We will develop a unified conceptual framework to model such single-molecule devices, treating these effects exactly and on an equal footing for the first time. We will also develop and perform state-of-the-art numerical simulations for quantum transport through realistic molecular junctions which we predict to realize novel functionality. Fundamentally, this research will address the challenge of how to harness the robust and reproducible chemical complexity provided by nature in single molecule devices.

Title: Gamma-ray bursts in the multi-messenger era

Supervisor: Dr Antonio Martin-Carillo (antonio.martin-carrillo@ucd.ie)

Gamma-Ray Bursts (GRBs) are intense flashes of gamma-rays that last from milliseconds to hundreds of seconds. They are the most powerful electromagnetic (EM) explosions in the universe, accelerating matter to near the speed of light in a narrow jet, producing the luminous flash of gamma-rays that allows these cosmic lighthouses to be seen back to the era of the first population of stars. 'Long' GRBs, lasting >2 seconds, are associated with the catastrophic core-collapse of supermassive stars into black holes. After the initial burst, a longer-lived afterglow is observed to radiate emitting from in radio-waves to X-rays, visible light and radio waves, which decays as a power-law with time. Coalescing binaries, thought to be the progenitors of the 'short' GRBs (<2 seconds), are widely viewed as the most promising gravitational wave (GW) candidate sources. The recent ground-breaking discovery of the first neutron star merger seen simultaneously as a short GRB and as a GW by LIGO/Virgo (GW170817) has opened up a new era of astrophysics confirming the nature of short GRBs and providing the best observation so far of a kilonova. GRBs and GWs are at the frontiers of astrophysics, playing a pivotal role in e.g. cosmology, stellar evolution, relativistic processes and formation of compact objects (black holes and neutron stars). The complex phenomenology of GRBs demands comprehensive space and ground-based multi-wavelength observations. The in-depth analysis required to contribute new understanding of these sources requires theoretical understanding, physical interpretation, computational modelling and data analysis.

Title: High definition sub-diffraction limited imaging using non-linear structured illumination

Supervisor: Associate Professor Dominic Zerulla (dominic.zerulla@ucd.ie)

Fluorescence microscopy is one of the most important key technologies for imaging of molecules, sub-cellular structures, and bio-medical processes in cells. However, it is limited by the Abbe diffraction limit of optics, namely a lateral resolution of λ/(2NA), where NA is the numerical aperture of the objective lens and λ is the wavelength of the emission light, limiting the attainable spatial resolution to ~200 nm for visible light.

Although this limit is a universal principle that cannot be broken directly, Structured Illumination Microscopy (SIM) is able to code high resolution information into the low resolution supported region of the microscope and thus circumvent the limit. The required additional information is generated in SIM by illuminating the object with a periodic pattern. The here described project is exploiting non-linear optical effects and surface bound evanescent waves to generate highly spatially confined illumination patterns in a precision interferometric device which will routinely yield super resolutions < 50 nm.

Title: High-Energy Studies of Active Galactic Nuclei

Supervisor: Associate Professor John Quinn (john.quinn@ucd.ie)

The High Energy Astrophysics Group has opportunities for projects entailing the study of Active Galactic Nuclei. The group is a founding member of the VERITAS collaboration, which operates an array of four imaging atmospheric Cherenkov telescopes in Arizona for very-high-energy (VHE) gamma-ray astronomy above 100 GeV, and is also participating in the CTA collaboration, which is constructing the next-generation of ground-based gamma-ray observatories. Projects utilising the VHE observations of blazars include combining the measurements with multiwavelength data from instruments such as Swift and Fermi-LAT, to constrain models of the emission processes in jets, and using the VHE data to study cosmological fields such as the extragalactic background light and the intergalactic magnetic field. The group is also a member of the I-LOFAR consortium that in 2017 installed an international LOFAR radio telescope station in Ireland. Opportunities for studying AGN with LOFAR include high resolution studies of select objects as well as surveys of many objects through the LOFAR AGN Survey group.

Title: Investigation of the double photoionization mechanism in aromatic hydrocarbons.

Supervisor: Associate Professor Emma Sokell (emma.sokell@ucd.ie)

http://www.ucd.ie/research/people/physics/assoc%20professoremmasokell/

Double photoionization (DPI) results in the emission of two electrons following the absorption of a single photon. DPI may be divided into direct and indirect processes and arises from electron-electron correlation. In indirect double photoionization, the process proceeds via resonant absorption of the photon to create an excited neutral [E. Sokell et al, Phys. Rev. Lett. **110,** 083001 (2013)] or singly ionized state, which subsequently decays to result in two electrons in the continuum and a doubly charged ion. Recently studies, in which the ratio of doubly charged to all parent ions was measured as a function of photon energy using time-of-flight spectroscopy, have revealed that a mechanism beyond the usual direct 'knock-out' mechanism is required to explain the data for aromatic hydrocarbons [R. Wehlitz et al, Phys. Rev. Lett. **109,** 193001 (2012)].

The aim of this project is to investigate double photoionization (DPI) in aromatic hydrocarbons, using angle-resolved and coincidence photoelectron spectroscopy. Specifically, a proposed new double photoionisation mechanism, involving Cooper pair formation in aromatic hydrocarbons due to their high degree of symmetry, will be explored by recording photoelectron-photoelectron coincidence spectra. These fully differential studies provide detailed information about the DPI process and will extend the previous work of Wehlitz et al.

There is a connection between aromatic hydrocarbons and graphene, and advances in the understanding of these molecules may have a bearing on our knowledge of unconventional superconductors including graphene.

Title: Probing electrochemical processes at the solid-liquid interface at the nanoscale with implications for energy materials and biological systems

Supervisor: Associate Professor Brian Rodriguez (brian.rodriguez@ucd.ie)

Whereas scanning electrochemical microscopy paved the way for current detection of electrochemistry at solid-liquid interfaces with microscale resolution, the exquisite force sensitivity of scanning probe microscopy (SPM) has yet to be harnessed to probe local electrochemistry phenomena at the nanoscale, despite extensive effort. We have recently developed electrochemical force microscopy (EcFM) to measure bias- and time-dependent electrochemical processes in liquid environments with nanoscale resolution. EcFM offers the potential to proble the fundamental physics of the solid-liquid interface to unravel the mechanisms of electron transfer and electrocatalysis – phenomena central to energy materials and biological systems.

There are several potential projects within this topic. Interested students can find more information in the paper below and are encouraged to contact Dr. Brian Rodriguez.

Further reading:

L. Collins, S. Jesse, J. I. Kilpatrick, A. Tselev, O. Varenyk, M. B. Okatan, S. A. L. Weber, A. Kumar, N. Balke, S. V. Kalinin, and B. J. Rodriguez, "Probing charge screening dynamics and electrochemical processes at the solid-liquid interface with electrochemical force microscopy," Nature Communications 5, 3871 (2014).

Title: Strong coupling in molecular exciton – plasmon array systems

Supervisor: Dr James Rice (james.rice@ucd.ie)

Developments in top-down and bottom-up nanofabrication techniques have enabled the development of active plasmonic nanomaterials such as arrays of gold nanorods with size- and shape-tunable plasmonic resonances [1,2]. Active plasmonics nanomaterials can be coupled with excitonic systems to give rise to hybrid plasmon–exciton modes (Plexcitons) when in the strong coupling regime [3-5]. Such systems when within the strong coupling limit effect changes in the optical processes of an emitter or absorber excitonic system. This offers potential to enhance or control exciton processes in excitonic systems such as organic semiconductors which offers opportunities for enhanced photonic device designs such as in light harvesting, optical sensing or artificial light sources. An understanding of light mater interactions of plasmon-exciton complexes is central in fully realizing the potential of such complexes.

A number of studies have demonstrated plasmon-exciton in the strong coupling limit between an organic exciton semiconductor and a surface plasmons and localized surface plasmons geometries. Studies have demonstrated that colloidal gold nanoshell-J-aggregate particles exhibit strong coupling between the localized plasmons of a nanoshell and the excitons of molecular J-aggregates adsorbed on its surface. The interaction of an organic exciton in a -aggregate and surface plasmon polariton modes of nanostructured hole arrays or of nanosize metallic disks with different array periods was reported to exhibit strong coupling. Tuning of plasmon–exciton coupling strength has been reported for strongly coupled exciton–plasmon states in Au nanodisk arrays coated with J-aggregate molecules achieved by changing the incident angle of incoming light, rather than changing the geometry of the plasmonic nanomaterial. Using such an angle resolved approach plasmon–exciton coupling of variable strengths was achieved.

We propose to demonstrate tuning/detuning of strong coupling in nanorod arrays achieved though angular tuning. Examining the properties of such systems. Assessing Rabi oscillations and fano resonances (induced transparency) through reflection and (ultrafast time-resolved) photoluminescence. In addition the examination of Raman scattering of materials under strong coupling. Assessing Raman enhancement through polariton states. [6] Examining the impact of magnetic and electric field effects on strong coupling.

References:

1) *Kabashin, A. V., P. Evans, et al. Nat. Material **8**, 867 - 871 (2009)*
2) *Damm, S., Fedele and J.H. Rice. Appl. Phys. Lett. **106**, 183109 (2015).*
3) *Barnes, W. L., Dereux, A., and T. W. Ebbesen, Nature **424**, 824 (2003).*
4) *Koenderink, A. F., Alù, A., and A. Polman. Science **348**, 516 (2015).*
5) *Purcell, E. M. Phys. Rev. **69**, 37 (1946).*
6) *Nagasawa, F et al. J. Phys. Chem. Lett., **5** (1),14–19 (2014)*

Title: The plasma physics of particle transport and acceleration at relativistic shocks

Supervisor: Professor Peter Duffy (peter.duffy@ucd.ie)

Observations of many high energy astrophysical sources such as gamma ray bursts and the jets from active galactic nuclei indicate the presence of highly relativistic flows and shock waves. These shocks and flows are sites for the acceleration of particles with energies above that of the background thermal plasma. The coupling between these high energy particles and the background plasma occurs via the excitation of waves. For example, the current associated with the high energy particles streaming ahead of the shock generates resonant and non-resonant waves in the upstream region. These, in turn, act to confine and scatter high energy particles back into the downstream region allowing the Fermi acceleration process to take place. The spectrum of the energetic particles is determined by the shock strength and nature of the scattering, and is well understood in the test particle limit. This project will examine the nature of the particle spectra beyond this test particle limit - where we look at the plasma physics of energetic particle acceleration and the turbulence that they generate in a self-consistent manner in relevant astrophysical shock waves and flows. There will be two complementary approaches (1) to construct and solve simplified kinetic models to look at this problem and (2) to use MHD simulations in relativistic flows with a high energy particle current included.

Further Reading:

1) *Rieger and Duffy 2016, "Shear acceleration in expanding flows", The Astrophysical Journal, Volume 483, Page 34 (http://adsabs.harvard.edu/abs/2016ApJ...833...34R)*

2) *Reville, Kirk and Duffy 2006, "A current-driven instability in parallel, relativistic shocks", Plasma Physics and Controlled Fusion, Volume 48, Page 1741 (http://adsabs.harvard.edu/abs/2006PPCF...48.1741R)*

Title: Theoretical and Computational Modeling of Dimerisation-Dependent Mechanisms on Molecular Signaling Pathways

Supervisor: Associate Professor Nicolae-Viorel (Vio) Buchete (buchete@ucd.ie)

In this project, we will develop computational molecular dynamics (MD) modeling and simulation methods to probe the conformational changes associated to protein-protein interactions involving proteins responsible of key signaling processes in biological cells. For example, the MST/Hippo pathway is a key, cancer-related signaling cascade, evolutionarily conserved, that controls crucial molecular processes including apoptosis (controlled cell death) in eukaryotic cells.

By using atomistic MD, we can now gain new understanding of the underlying chemical biophysics, by combining recent experimental information (X-ray crystallography) and systems biology studies with recent advances in accurate MD-based techniques. This approach could lead to the development of new drugs (e.g., aimed at new types of anticancer drug targets), as well as to new drug candidates that selectively interact along signaling pathways.

Using experimental information, we will simulate structural models of kinase-kinase homo- and hetero dimers using multiple representation scales, from atomistic to coarse-grained residue-level models. These data will allow us to infer the minimal models that could capture accurately the underlying statistical and biophysical mechanisms of these complex molecular systems.

To overcome the system size-related challenges in MD, we will continue to develop and use state-of-the-art Markov model-based enhanced sampling and optimization methods. Depending on the system, a variety of enhanced sampling techniques, from replica exchange to umbrella sampling and equilibrium sets of short trajectories will be employed.

Further reading:

1. *Martini, Kells, Covino, Hummer,* ***<u>Buchete</u>*** *and Rosta, "Identification and Analysis of Transition and Metastable Markov States" (**2017**), Phys. Rev. X.,* ***7*** *(3):031060 (2017 (arXiv:1605.04328)*
2. *Leahy, Murphy, Hummer, Rosta, and* ***<u>Buchete</u>****, "Coarse Master Equations for Binding Kinetics of Amyloid Peptide Dimers. J Phys Chem Lett* ***7****, 2676-2682 (**2016**).*
3. *Sanchez-Sanz, Tywoniuk, Matallanas, Romano, Nguyen, Kholodenko, Rosta, Kolch, and* ***<u>Buchete</u>****, "SARAH Domain-mediated MST2-RASSF Dimeric Interactions" PLoS Comput Biol* ***12****, e1005051, doi:10.1371/journal.pcbi.1005051 (**2016**).*