

# **DEPARTMENT OF PHYSICS**

# Fourth Year Research Projects 2014/15 Second Round

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# **Health and Safety**

Undergraduate students need to undergo appropriate safety training for their projects. The University Occupational Health & Safety Arrangements state:

#### 16.4 Supervision of Students

- Departments recognise that most undergraduate students are initially untrained in matters of health and safety, therefore, Academics will provide information, instruction, training and "such supervision as is necessary", for all aspects of coursework, to ensure, so far as is reasonably practicable, the health and safety of both postgraduate and undergraduate students;
- Coursework will cover, practical work, project work, fieldwork, work placements and any other aspect required of students by their courses;
- Departments will record the means of delivery of the health and safety programme for each course, each year;
- Academic Supervisors will determine the appropriate level of supervision, based on an
  assessment of risks of the research or teaching activity etc. and documented training received
  by students; Academic Supervisors will personally provide necessary supervision, unless others
  are identified by the relevant risk assessment.

An Undergraduate safety induction training record is required to be completed for each project student. Please ensure that the training is completed and the form returned to Lynn Gilmour before the project work begins. (see Appendix 1)

With thanks,

Mr Ron Weston

**Nanoscience Division** 

# **Predicting Solvation Thermodynamics of Bioactive Molecules**

Project Supervisors: (1) Prof Maxim V. Fedorov, (2) Dr Neil Hunt & Dr David Palmer

# **Project Description:**

The project will study solvation thermodynamics of bioactive molecules by novel computer modelling methods.

One of the main causes of the unacceptable attrition rate in drug discovery is the failure of molecules to reach the market place because they have the wrong physico-chemical properties to allow them to be orally administered to patients. Indeed, as many as 40% of all drug failures on the market have been attributed to these problems.

Experimental high-throughput measurements of physico-chemical properties of bioactive molecules (solubility, pKa, logP, etc) are traditionally used to screen candidate drug molecules. However, such experiments are expensive, time-consuming and can only be applied to molecules that have already been synthesized. An alternative approach is to use computer simulations to calculate the properties of putative drug molecules.

Recently we developed a highly efficient method for predicting solvation thermodynamics parameters of bioactive molecules in a view of potential medical and environmental applications. The method is based on a molecular theory of solutions, Reference Interaction Sites Model (RISM). The student will have the opportunity to be involved into large-scale computational screening of thermodynamic properties of drug-like molecules and agrochemicals by this new method.

**Reference:** Kerns, E. H. & Di, L. (2008), Drug-like properties: concepts, structure design and methods: from ADME to toxicity optimization, Academic Press;

Additional references will be provided.

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 30% Comp: 70%

**Suitability:** MPhys, BSc

**Additional comments:** Suitable for Masters-level students with good computer skills and an interest in chemical/molecular physics or biophysics. This is an excellent opportunity for students to get experience in novel state-of-the-art methods of molecular modelling.

# Molecular Mechanisms of Biological Adaptation to Extreme Ionic Environments

Project Supervisors: (1) Prof Maxim V. Fedorov, (2) Dr Neil Hunt & Dr David S. Palmer

# **Project Description:**

The project will study molecular mechanisms of protein resistance to extreme ionic environments by use of different methods of experimental and computational molecular biophysics.

Among different types of life there is one that exists under conditions considered for a long time as a dead zone. These living (micro) organisms are called "extremophiles". They feel comfortable at such extreme conditions as high (>70° C) temperatures (thermophile), extreme pH (alkaliphile, acidophile), high salinity (halophile) etc.

In the current project we will study molecular structures of enzymes from *halophilic bacteria* that inhabit hypersaline environments such as those found in the Dead Sea and saltern evaporation ponds. It was found that such aggressive media where 'normal' organisms cannot survive are the optimum living conditions for the halophilic species. During the billions years of evolution, the halophilic organisms developed *molecular mechanisms* of adaptation to highly concentrated salt environments. However, these mechanisms are still poorly understood. There are several hypotheses for the main mechanisms of halophilic proteins resistance to extreme ionic environments: (i) accumulation of negative charges on the protein surface; (ii) minimization of the solvent accessible surface area.

The main goal of the study will be to explore correlations between the surface charge and the surface area of different mutants of halophilic proteins compared to their homologous counterparts from 'normal' organisms. The project will involve experimental spectroscopic studies of polypeptides/proteins and homologous molecular modelling of proteins and structural analysis of the protein structures.

**Key References:** Gross M. "Life on the Edge: Amazing Creatures Thriving in Extreme Environments", New YorK: Plenum (1998); Lesk, A. M. "Introduction to protein architecture", Oxford (2001); SWISS-MODEL Protein Modelling Environment (http://swissmodel.expasy.org); additional references will be provided.

Ratio of effort: Exp/Theo/Comp Exp: up to 50%

Theo: 10% Comp: 40-70%

**Suitability:** MPhys, BSc

**Additional comments:** Suitable for students at all levels with good computer skills and an interest in molecular biophysics. The student will get experience in modern state-of-the-art tools of protein structural analysis and bioinformatics applications in molecular biophysics.

# Ionic Liquids at Charged Interfaces: Applications for Electrochemical Energy Storage

Project Supervisors: (1) Prof. Maxim V. Fedorov, (2) Dr Yu Chen

# **Project Description:**

The project is focused on the theoretical modelling of ionic liquids (IL) and electrified interfaces (ES). Ionic liquids are strongly believed to replace traditional electrolytes in high efficiency electrochemical devices for energy storage and transformation (e.g supercapacitors), due to their superior physicochemical properties, especially very low volatility and high electrochemical stability.

High-resolution modelling of the structure of ILs near the electrode surface is crucial for the understanding of electrochemical processes in RTILs. The results of the project would serve as a basis for understanding and rationalising the structure—potential and structure—property dependence of the electrified interface between ionic liquids and charged surface.

The main task of the project is to apply methods of Quantum Mechanics and Molecular Mechanics methods to investigate ILs at ES. The student will get experience with High Performance Computing (HPC) applications in chemical physics and theoretical/computational description of IL-based supercapacitors and batteries. The computational part of the project will be done with use of the ARCHIE-WeST HPC facilities (www.archie-west.ac.uk).

**Key Reference (if applicable): M.V. Fedorov** and A.A. Kornyshev (2014). Ionic liquids at electrified interfaces. // *Chemical Reviews*, **114**(5), 2978.

Ratio of effort: Exp/Theo/Comp Exp: 0 %

Theo: 50 % Comp: 50 %

Suitability: MPhys, BSc, BSc (Phys with Teaching), BSc (Maths Physics)

**Additional comments:** Solid background in theoretical physics and statistical mechanics is strongly required. Some experience with computations and/or data analysis would be a plus.

# Development of Molecular-scale Computer Models for Enhanced Oil Recovery

Project Supervisors: (1) Prof Maxim V. Fedorov, (2) Dr Neil Hunt

## **Project Description:**

The project is a part of ongoing collaboration with Schlumberger and it is focused on development of advanced molecular-scale models for enhanced oil recovery (EOR). Waterflooding is widely applied to boost declining oil reservoir pressure and sweep additional oil into production wells. Success in waterflooding is a key element to improved oil recovery.

In this project we intend to develop new computational model based on Molecular Dynamics for predicting and understanding characteristics of aqueous brines used for waterflooding in oil/gas reservoirs and complex mixtures of these brines with organic compounds. To facilitate this, a number of fundamental phenomena need to be understood by use of large-scale supercomputer simulations such as thermodynamics of ion solvation in brines; physico-chemical properties of brines at high temperature and pressure; the role of ions and counter-ions such as naturally occurring in sea water and ion effects on structural and thermodynamic properties of organic (bio)molecules.

The student will get experience with High Performance Computing (HPC) applications in chemical physics and use of HPC in development of advanced EORs. The computational part of the project will be done with use of the ARCHIE-WeST HPC facilities (www.archie-west.ac.uk).

**Key Reference (if applicable):** (book) Israelachvili, J.N., 2011. Intermolecular and surface forces. Academic Press, Burlington, MA. (book) Frenkel, D., Smit, B., 2002. Understanding molecular simulation. Academic Press.

Ratio of effort: Exp/Theo/Comp Exp: 0 %

Theo: 50 % Comp: 50 %

**Suitability:** MPhys, BSc, BSc (Phys with Teaching), BSc (Maths Physics)

**Additional comments:** Solid background in theoretical physics and statistical mechanics is strongly required. Some experience with computations and/or data analysis would be a plus.

# Modelling of Wettability of Mineral Surface by Water and Oil

# Project Supervisors: (1) Prof. Maxim V. Fedorov, (2) Dr Yu Chen

# **Project Description:**

The project is a part of ongoing collaboration with Schlumberger and it is focused on development of advanced molecular-scale models for understanding wettability of mineral (calcite) surface by water and hydrocarbons. Waterflooding is widely applied to boost declining reservoir pressure and sweep additional oil into producing wells. Success in waterflooding is a key element of Enhanced Oil Recovery (EOR) techniques. Specific interactions between crude oil/water/rock can lead to large variations in the displacement efficiency of water floods. The rock wettability by reservoir fluids affects not only the release of heavy ends of crude oil, but also the attachment of fine solids, e.g. clays, to the liberated mineral surface. Fundamental understanding of the wettability of mineral solids from oil reservoir could substantially enhance the efficiency of oil recovery.

In this project we intend to develop new computational model based on Molecular Dynamics for predicting and understanding interfacial properties of mineral-water-hydrocarbon systems. We aim to rationalize the wettability mechanism of the mineral surface by atomistic simulations of the rock/oil and rock/water interfaces.

The student will get experience with High Performance Computing (HPC) applications in chemical physics and theoretical/computational description of mineral/water and mineral/oil systems important for the oil & gas sector. The computational part of the project will be done with use of the ARCHIE-WeST HPC facilities (www.archie-west.ac.uk).

**Key Reference (if applicable):** (book) Israelachvili, J.N., 2011. Intermolecular and surface forces. Academic Press, Burlington, MA. (book) Frenkel, D., Smit, B., 2002. Understanding molecular simulation. Academic Press.

Ratio of effort: Exp/Theo/Comp Exp: 0 %

Theo: 50 % Comp: 50 %

**Suitability:** MPhys, BSc, BSc (Phys with Teaching), BSc (Maths Physics)

**Additional comments:** Solid background in theoretical physics and statistical mechanics is strongly required. Some experience with computations and/or data analysis would be a plus.

# **Effects of Salts on Surfactant Solutions**

# Project Supervisors: (1) Prof. Maxim Fedorov, (2) Dr Neil Hunt

#### **Project Description:**

The project is focused on molecular-scale simulations of effects of ions on the stability of surfactant solutions. Aqueous surfactant solutions are widely used in many industries; however, we are particularly interested in surfactants used for enhanced oil recovery (EOR).

In this project we will use Molecular Dynamics simulations for understanding molecular-scale effects of dissolved inorganic salts on stability of aqueous surfactant solutions. We plan to use large-scale supercomputer simulations to investigate thermodynamics of ion and surfactant solvation in water; physico-chemical properties of surfactant/salt solutions at high temperature and pressure; the role of ions and counter-ions such as naturally occurring in sea water and ion effects on the phase diagram of surfactant solutions.

The student will get experience with High Performance Computing (HPC) applications in chemical physics and use of HPC in development of advanced EORs. The computational part of the project will be done with use of the ARCHIE-WeST HPC facilities (www.archie-west.ac.uk).

**Key Reference (if applicable):** (book) Israelachvili, J.N., 2011. Intermolecular and surface forces. Academic Press, Burlington, MA.

(book) Frenkel, D., Smit, B., 2002. Understanding molecular simulation. Academic Press.

Ratio of effort: Exp/Theo/Comp Exp: 0 %

Theo: 50 % Comp: 50 %

**Suitability:** MPhys, BSc, BSc (Phys with Teaching), BSc (Maths Physics)

**Additional comments:** Solid background in theoretical physics and statistical mechanics is strongly required. Some experience with computations and/or data analysis would be a plus.

# **Predicting Small Molecule Binding Sites on Protein Surfaces**

# Project Supervisors: (1) Prof. Maxim Fedorov, (2) Dr David Palmer

# **Project Description:**

Binding of small molecules (ligands) by proteins plays very important role in biology. In fact, protein-ligan binding is the main mechanism of regulation of complicated in vivo and in vitro biochemical reactions. Therefore, protein-ligand binding studies play very important role in many areas of biotechnology and drug development & design.

However, direct experiments on protein-ligand systems are laborious and expensive; moreover, experimental measurements do not provide direct information about molecular-scale mechanisms of binding. In addition, for many important protein systems (e.g. membrane proteins) direct experiments are hardly possible these days due to problems with protein purification and stabilization. Therefore, molecular modeling plays important role in these studies as a complimentary tool to experimental techniques.

The main goal of the project is to apply advanced modeling techniques developed by Fedorov & Palmer together with their co-workers to the problem of predicting small molecule binding sites for a selected set of proteins.

The core of the method is the so-called 3D Reference Interaction Site Model (3D-RISM) that allows one to calculate 3D distributions of different small molecules (as well as water) near the protein surface. If successful, the expected results of the projects may have important applications in pharmacology and biotechnology areas.

**Key References:** D.S. Palmer, A.I. Frolov, E.L. Ratkova and M.V. Fedorov (2011). Towards a Universal Model to Calculate the Solvation Thermodynamics of Druglike Molecules: The Importance of New Experimental Databases. // Molecular Pharmaceuticals, 8, 1423-1429. Lesk, A. M. "Introduction to protein architecture", Oxford (2001); SWISS-MODEL Protein Modelling Environment (http://swissmodel.expasy.org); Additional references will be provided.

Ratio of effort: Exp/Theo/Comp Exp: 70%

Theo: 10% Comp: 20%

**Suitability:** MPhys, BSc, BSc (Phys with Teaching), BSc (Maths Physics)

**Additional comments:** Some knowledge of programming/scripting languages and Linux (Unix) OS would be a plus.

# Thermal Modelling of a Gravitational Ribbon Sensor

Project Supervisors: (1) Dr Nicholas Lockerbie, (2) Dr Wayne McRae

# **Project Description:**

Gravity gradiometers measure the change in the Earth's gravitational field over the length of a sensing element or elements. Some common methods used for practical gradiometers include matched accelerometers connected in a differential configuration, or measuring the deflection of a very precise torsion balance. Because gravity is by its very nature a weak force, and the subtle changes in the force are many times smaller than the dominant uniform field on Earth, great care must be taken in the development of any commercial gravity gradiometer.

This project covers modelling the temperature response of the ribbon gravity gradiometer sensor and determining methods to improve thermal performance. This work will include theoretial and modelling using FEA software as well as experimental work to validate the modelled results. The student should be willing to learn to use FEA modelling software.

## **Key Reference:**

http://www.gravitec.co.nz/publications.html (Gravity Gradiometer Publications)

Ratio of effort: Exp/Theo/Comp Exp: 30%

Theo: 30% Comp: 40%

**Suitability:** BSc, BSc Maths and Physics

**Additional comments:** The student should be willing to learn CAD and FEA modelling techniques and should be familiar with Matlab.

# **Gravitational Ribbon-Sensor Modelling**

# Project Supervisors: (1) Dr Nicholas Lockerbie, (2) Dr Wayne McRae

#### **Project Description:**

Gravity gradiometers measure the change in the Earth's gravitational field over the length of a sensing element or elements. Some common methods used for practical gradiometers include matched accelerometers connected in a differential configuration, or measuring the deflection of a very precise torsion balance. Because gravity is by its very nature a weak force, and the subtle changes in the force are many times smaller than the dominant uniform field on Earth, great care must be taken in the development of any commercial gravity gradiometer.

The design of the ribbon sensing element has a significant effect on the performance of the sensor. The focus of the project is to optimise and test designs, including FEA modelling of response to gravity loading. Successful designs will be manufactured and tested in the lab to measure performance relative to sensor requirements. The student should be willing to learn to use FEA modelling software.

#### **Key Reference:**

http://www.gravitec.co.nz/publications.html (Gravity Gradiometer Publications)

Ratio of effort: Exp/Theo/Comp Exp: 30%

Theo: 30% Comp: 40%

Suitability: BSc, BSc Maths and Physics

**Additional comments:** The student should be willing to learn CAD and FEA modelling techniques and should be familiar with Matlab.

# Laser Selective Excitation Studies of Nd<sup>3+</sup> Doped Mixed Garnets

Supervisors (1) Dr Thomas Han, (2) TBA

#### **Project Description**

(This project can accommodate 2 students each studying a different aspect of the garnet host.)

When trivalent rare-earth ions are introduced into a crystal lattice substituting for divalent cation some form of charge compensation is required for the crystal to maintained charge neutrality. A wide variety of symmetry configurations can be produced depending on the charge compensator(s) and the rare-earth ion(s) in the host lattice. Selective laser excitation technique can be used to determine the site distribution and symmetry of the various centres in the crystal. The aim of this project is to investigate the spectroscopic properties of garnet crystals doped with different concentrations of rare-earth ion. This project is a continuation of part of a Phd investigation of Nd<sup>3+</sup> doped in a series of mixed garnets. The aim is to investigation the effect of local environment disordering has on the optical properties of the active ions. The main effect is inhomogeneous broadening of the spectral linewidth which has the potential for shorter pulse generation. This project involves a detail LSE study of a specially selected subset of mixed garnets aiming to resolve the inhomogeneously broadened spectral lines and to investigate 'new' defect centres. The project involves the use of technique such as optical absorption, laser spectroscopy and fluorescence decay measurements.

#### **Key Reference (if applicable):**

L. A. Riseberg , R. M. Brown , and W. C. Holton, Applied Physics Letters 23 , 127 (1973); doi: 10.1063/1.1654830

Ratio of effort: Exp/Theo/Comp Exp: 85%

Theo: 10% Comp: 5%

**Suitability:** MPhys and BSc

#### Additional comments:

Garnet is a well-studied laser gain material and there are plenty of literatures on the properties of rare-earth ion doped garnets. However, aspects of this project require patient and lots of laboratory time. You should be interested in experimental work and will be working with lasers.

Safety Training Requirements: General laboratory and Laser safety

# Stimulated Raman Spectroscopy (SRS) of Organic Liquids

# Project Supervisors: (1) Dr Thomas Han, (2) Dr David McKee

#### **Project Description:**

Raman scattering is an inelastic collision between a photo and a molecule (or particle). Because of energy conservation, the inelastic collision results in absorption of the photon and generation of another photon at different wavelengths. The shift of photon wavelength can be a positive or negative value, which leads to a Stokes or an anti-Stokes transition, respectively. At a high power of stimulated photon intensity, stimulated-raman scattering (SRS) can produce a new type of wavelength tunable laser. Raman lasers have been extensively studied in active media of solids, liquids and gases. The key objectives of this project are to study the SRS of a raman active organic liquid such as DMSO or acetone and investigate the efficient, stability and tunability of such a system.

## Key Reference (if applicable):

F.G. Yang, Z.Y. You, Z.J. Zhu, Y. Wang, 1 J.F. Li, C.Y. Tu, Laser Phys. Lett. 7, (2010) 14.

Y.S. Cheng, J.G. Yang, M.H. Chan, Chin. Phys. Lett. <u>23</u>, (2006) 135.

Ratio of effort: Exp/Theo/Comp Exp: 85%

Theo: 10% Comp: 5%

**Suitability:** MPhys, BSc

#### **Additional comments:**

This is a relatively speculative project that positive results may be difficult to obtain but other researchers have shown promising results. Aspects of this project require patient and lots of laboratory time. You should be interested in experimental work and will be working with lasers and chemicals.

Safety Training Requirements: General laboratory and Laser safety

# **Optical Modes and Multiple Scattering**

# Project supervisors: (1) Dr Ben Hourahine (2) Dr Francesco Papoff

# **Project Description:**

It has recently been shown that the optical properties of most nano-particles can be understood as arising from the modes of the particle. These are, like the standing acoustic waves of an organ pipe or the wavefunctions of a quantum mechanical particle in a box, distinct solutions of the appropriate wave equations (here, Maxwell's equations). However, if a second particle is brought close by, how does this affect these modes?

Light will then "bounce" between these two particles (multiple scattering), leading to a new set of optical modes which describe the whole composite system. This project will theoretically and computationally study the transition between the isolated and coupled modes of two glass particles as they approach each other.

#### **Key Reference (if applicable):**

F. Papoff, B. Hourahine, Geometrical Mie theory for resonances in nanoparticles of any shape, Optics Express, 19, 21432 (2011)

Ratio of Experiment/Theory/Computation: Exp = 0%,

Theo = 50%, Comp = 50%

Suitability: MPhys, BSc

# **Twisted Nanostructures**

# Project supervisors: (1) Dr Ben Hourahine (2) Prof. Maxim Fedorov

#### **Project Description:**

In addition to the familiar arrays of atoms in crystals, there are several other types of large ordered arrangements of atoms which occur in nature which are not periodic. For example there are many structures that are fundamentally helical in nature, these include carbon nanotubes, screw-dislocated nanowires, the tails and capsids of many viruses, amyloid fibrils, and perhaps most famous, DNA. Traditionally these are investigated by either using large clusters of atoms to describe segments of the helical structure, or as a crystal with a large number of atoms in its unit cell to include a complete twist of the helix. Both of these approaches require the simulation of very many atoms, even though the fundamental repeat unit of the structure is often much smaller.

This project applies the recently developed idea of simulating this fundamental repeat unit (the so called 'objective' cell) to study twisted nanostructures. Potential systems to be studied in this project are helical carbon nanotubes, twisted semiconductor nanowires or the DNA helix.

#### **Key Reference (if applicable):**

D.-B. Zhang, M. Hua, and T. Dumitrica, J. Chem. Phys. 128, 084104 (2008).

Ratio of Experiment/Theory/Computation: Exp = 0%,

Theo = 30%, Comp = 70%

**Suitability:** MPhys, BSc

# Noise and System Response of CCD Spectrographs for Luminescence Spectroscopy

Project Supervisors: (1) Dr Paul Edwards, (2) Prof. Robert Martin

#### **Project Description:**

Charge-coupled device (CCD) detectors have transformed many areas of scientific research, allowing optical spectra to be collected rapidly and with high signal-to-noise ratios. This project will examine limiting factors in the signal-to-noise ratio of luminescence spectroscopy measurements carried out using CCD spectrographs. The response of such systems is a strong function of both wavelength and polarization, and the project will investigate these aspects both theoretically and through experimental measurements. CCD noise will be quantified with the aim of determining which factors dominate under typical measurement conditions (e.g. during the acquisition of a cathodoluminescence hyperspectral image). The relative influence of shot noise (Poissonian) and read-out noise (Gaussian) will be compared for different sensors: not only conventional CCDs but also electron-multiplying (EMCCD) and image-intensified (ICCD) variants. The project may also be broadened to include the implications of the noise distribution for the pre-treatment of data prior to the application of multivariate statistical analysis methods.

#### **Key Reference:**

M. Lesser, "Charge coupled device (CCD) image sensors", in High Performance Silicon Imaging, edited by Daniel Durini, Woodhead Publishing, 2014, Pages 78-97, 10.1533/9780857097521.1.78

P. R. Edwards, L. Krishnan Jagadamma, J. Bruckbauer, C. Liu, P. Shields, D. Allsopp, T. Wang, R. W. Martin (2012) *Microscopy and Microanalysis* **18** 1212–1219 10.1017/S1431927612013475

Ratio of effort: Exp/Theo/Comp Exp: 50%

Theo: 25% Comp: 25%

Suitability: MPhys, BSc, BSc Maths and Physics, BSc Physics with Teaching

**Additional comments:** 

# **Luminescence Hysteresis**

# Project Supervisors (1) Prof. Kevin O'Donnell, (2) Dr Paul Edwards

# **Project Description:**

The Semiconductor Spectroscopy group recently discovered luminescence hysteresis in the optical spectra of europium-doped GaN. We are currently investigating this new phenomenon with a view to elaborating a tentative explanation of it, in the area of solid state defect physics, as described in the Key (and only!) Reference below.

Hysteresis is generally a consequence of *path dependence* in physical processes. In the present case, the luminescence spectrum of Eu-doped p-type GaN at a given temperature depends upon the sample's thermal history. The measured spectrum will be different, for example, if the sample is cooled from room temperature to the measuring point or warmed from low temperature to that point.

The project will examine the dynamics of the process leading to hysteresis in this case, using a fast CCD camera to acquire luminescence spectra as a function of sample history. For this we will need to collect and analyse quite a lot of data, providing an excellent opportunity for a student who are is attracted by laboratory work and is good with computers, used in particular for data handling and reduction

**Key Reference (if applicable):** "Temperature-Dependent Hysteresis of the Emission Spectrum of Euimplanted, Mg-doped HVPE GaN" by K.P. O'Donnell et al.

Proceedings of the 31st International Conference on the Physics of Semiconductors. (Zurich, 2012)

Ratio of effort (Exp/Theo/Comp): Exp: 50%
Theo: 10%

Theo: 10% Comp: 40%

Suitability: MPhys, BSc

**Additional comments:** 

**Safety Training Requirements:** some laser spectroscopy may be required.

**Optics Division** 

# **Beam Quality of Broad-area Diode Lasers**

# Project Supervisors: (1) Prof. Thorsten Ackemann, (2) Dr Michael Strain

# **Project Description:**

Power scaling of semiconductor laser diodes and maintaining at the same time a high beam quality is a notoriously difficult challenge, since increasing the emission aperture leads to numerous instabilities limiting the brightness of a broad-area laser (BAL) [2].

Recently, a novel approach to control the beam quality of edge-emitting BALs maintaining their attractive monolithic compactness was proposed [1]. The suggestion is to implement a two-dimensional spatial modulation- *simultaneously transverse and parallel to the cavity axis* — of the gain characteristics, i.e. of the imaginary part of the susceptibility, by a modulation of the current injection. Similar to the case of photonic crystals (relying on a modulation of the real part of the susceptibility), the modulation is predicted to lead to a modification of spatial dispersion curves, in particular to a spatial filtering and a highly directional gain along the optical axis. As a result, *noise triggered by inhomogeneities or dynamically generated via instabilities* is quenched.

The project will set up a probe station to measure beam quality of BALs and perform measurements of samples processed at the University of Glasgow.

**Key Reference:** [1] R. Herrero et al., Beam shaping in spatially modulated broad-areasemiconductor amplifiers, Opt Lett. 37, 5253 (2012); [2] Crump et al., Experimental and theoretical analysis of the dominant lateral waveguiding mechanism in 975 nm high power broad area diode lasers. Semicond. Sci. Technol. **27** (2012) 045001

Ratio of effort: Exp/Theo/Comp Exp: 70%
Theo: 10%

Comp: 20%

Suitability: MPhys, BSc

**Additional comments:** The student is required to attend PH445 and PH453 to obtain the necessary background.

**Safety Training Requirements:** laser

# Characterization of Optically pumped Quantum Well and Quantum Dot Vertical-cavity Structures

Project Supervisors: (1) Prof. Thorsten Ackemann, (2) Dr Antonio Hurtado

## **Project Description:**

The research field of spintronics aims at utilizing the carrier spin for applications in addition to the number of carriers as usual in electronics and semiconductor photonics. However, electrical injection of spin polarized carriers is still limited to cryogenic temperatures or low temperatures in combination with a large magnetic field. At room temperature, optical pumping provides a convenient alternative to electrical injection since carrier spin and photon spin are coupled by angular momentum selection rules. III-V semiconductor gain media in vertical-cavity structures possess the necessary isotropy in the plane of the gain medium to investigate spin dependent effects. Most work centred on relatively low gain structures in vertical-cavity surface-emitting lasers (VCSEL) with quantum well gain media.

This project will look at high gain quantum well samples for external-cavity use (VECSELs) and VCSEL structures containing quantum dots, zero dimensional semiconductors with quantum confinement in all directions. The measurements will start with analyzing the polarization properties of the photoluminescence in dependence on the polarization ellipticity of the optical pump field. Polarization dependent gain will be measured afterwards via a tunable laser. The final aim of the project is to achieve lasing.

#### **Key Reference (if applicable):**

Bhattacharya et al., Quantum dot polarized light sources, Semicond. Sci. Technol. 26 (2011) 014002

Hoevel et al., Appl. Phys. Lett. 92, 041118 (2008)

Ratio of effort: Exp/Theo/Comp Exp: 70%

Theo: 15% Comp: 15%

**Suitability:** MPhys BSc

Additional comments: The student is required to attend PH445 and PH453 to obtain the necessary

background.

Safety Training Requirements: Laser safety

# **State Comparison Amplification of Schrodinger Cats**

# Project Supervisors: (1) Dr John Jeffers, (2) Dr Marco Piani

# **Project Description:**

The state comparison amplifier is a simple means of producing a higher amplitude coherent state from a lower one. The device uses only beam splitters, detectors and a laser.

Quantum optical Schrodinger cats are superpositions of different coherent states of light, and are notoriously fragile. Their possible applications in quantum information render them extremely useful, despite them being a difficult-to-produce quantum resource.

This project will describe the possible means of increasing the amplitude of Schrodinger cats, rendering them less susceptible to loss.

# **Key Reference:**

Quantum Optical State Comparison Amplifier, E Eleftheriadou, SM Barnett, J Jeffers, Physical Review Letters 111 (21), 213601, (2013)

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 60% Comp: 40%

**Suitability:** MPhys, BSc, BSc Maths and Physics

**Additional comments:** Students should have passed well (~70%) third year quantum physics. Attendance at Quantum Optics and/or Quantum Information Classes would be desirable.

# **Quantum Measurement in the Jaynes-Cummings Model**

Project Supervisors: (1) Dr Daniel Oi, (2) Dr John Jeffers

#### **Project Description:**

Measurement plays a vital role in quantum information theory. Non-destructive measurement of optical fields is challenging to implement. One method is to couple a two-level atom to a cavity mode and through the interaction extract information from the field via the atomic state. Due to bosonic enhancement, the resulting measurement operators can be complicated and this project will investigate the resulting cavity dynamics.

#### **Key Reference:**

Nondemolition measurement of the vacuum state or its complement, D.K.L. Oi, V. Potoček, J. Jeffers, Physical Review Letters **110**, 210504 (2013)

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 50% Comp: 50%

Suitability: MPhys, BSc, BSc Maths and Physics, BSc Physics with Teaching

**Additional comments:** 

# **Ancilla-driven Quantum Dynamics**

# Project Supervisors: (1) Dr Daniel Oi, (2) Dr Marco Piani

# **Project Description:**

The ability to perform information processing tasks using quantum systems depends on the resources available. In the Ancilla Driven Quantum Computation model, the main resource is a single two-qubit unitary interaction that can drive evolution of a system via coupling to an ancilla. By suitable preparation and measurement of the ancilla, different effects can be applied to the system, but this depends on the form of the interaction. This project would investigate the relationship between the form of the unitary and what can be achieved.

#### **Key Reference:**

Ancilla-driven universal quantum computation, J. Anders, D.K.L. Oi, E. Kashefi, D.E. Browne, E. Andersson, Physical Review A **82**, 020301 (2010)

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 90% Comp: 10%

Suitability: MPhys, BSc, BSc Maths and Physics, BSc Physics with Teaching

**Additional comments:** 

# Spiral Bandwidth Control in Optical Parametric Oscillators

# Project Supervisors: (1) Dr Alison M Yao, (2) Prof. Gian-Luca Oppo

#### **Project Description:**

Optical parametric oscillators (OPOs) consist of a nonlinear crystal placed inside an optical cavity. The crystal converts a pump photon into two lower-frequency photons via a process known as spontaneous parametric down conversion (SPDC), while the cavity amplifies the down-converted beams by resonating either one (singly resonant) or both (doubly resonant) of the output beams. Doubly resonant optical parametric oscillators have been shown to produce signal and idler output beams that can have different amounts of orbital angular momentum (OAM). The range of OAM found in the output is known as the spiral bandwidth (SB) [1].

For quantum communication purposes, it is desirable to maximise the SB. In SPDC alone, the SB can be increased by changing the ratio of the pump width to the signal/idler width. In current OPO models, however, it is not possible to change this ratio as there is no control over the signal/idler size. The aim of this project is to incorporate curved mirrors into the simulations of OPO cavities [2]. By changing the radius of curvature of these mirrors the size of the signal/idler beam on the nonlinear crystal can be controlled. In this way we hope to develop a means of controlling the SB in widely used devices for the generation of entangled photons.

#### **Key Reference (if applicable):**

[1] A. M. Yao, "Angular momentum decomposition of entangled photons with an arbitrary pump", New J. Phys. **13**, 053048 (2011).

[2] M. Santagiustina, E. Hernandez-Garcia, M. San-Miguel, A. J. Scroggie and G.-L. Oppo, *Phys. Rev. E* **65**, 036610 (2002).

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 30% Comp: 70%

**Suitability:** MPhys BSc (Maths Physics)

Additional comments: The project requires skills in mathematical and computational techniques.

# **Resonances in Clouds of Cold Atoms**

# Project supervisors: (1) Dr Francesco Papoff (2) Dr Gordon Robb and Dr Ben Hourahine

#### **Project Description:**

Spherical clouds of cold atoms and Bose-Einstein condensate have electromagnetic resonances that are similar to the Mie resonances of spherical dielectric particles. In most experiments, however, the atomic clouds are more similar to elongated cigars than to spheres. In this project we will develop a theory for bodies with axially symmetric density that will apply to these experiments and we will consider whether the scattering of light from these clouds can become an effective diagnostic tool to measure the density of the cloud.

Ratio of Experiment/Theory/Computation: Exp 0%

Theo 50% Comp 50%

Suitability: MPhys, BSc

# Fluctuations and Noise in Cold Atoms

# Project supervisors: (1) Dr Francesco Papoff (2) Dr Gordon Robb

#### **Project Description:**

Noise plays a crucial role in all physical systems and in many cases it is not an hindrance, but an essential ingredient for the observation of processes as important as laser emission, for instance. In this project we will investigate theoretically and numerically the nature of small noisy fluctuations present in cold atoms interacting with coherent light, a very important system where it is possible to observe collective phenomena, linear and non-linear behaviour and many types of instabilities. In particular, we will find how noisy perturbations affect the the collective behaviour of cold atoms and explore regimes where they are be amplified.

**Key Reference (if applicable):** http://sbfel3.ucsb.edu/www/vl\_fel.html

F. Papoff, G. D'Alessandro, G.-L. Oppo, Phys. Rev. Lett. 100, 123905, 1-4, (2008)

F. Papoff, G.R.M Robb, Phys. Rev. Lett. 108, 113902 (2012)

Ratio of Experiment/Theory/Computation: Exp = 0%,

Theo = 50%, Comp = 50%

Suitability: PH450 MPhys BSc

**Additional Comments:** 

# **Dynamics of Coupled Laser Systems**

# Project Supervisors: (1) Prof. Gian-Luca Oppo, (2) Prof. Thorsten Ackemann

# **Project Description:**

It is well known that coupled lasers can synchronise by locking their phases when the coupling strength is large enough. Two typical examples of coupled laser systems are lasers injecting each other and closely placed laser waveguides. This project investigates and compares the dynamics of these two systems before and after the locking threshold when increasing the coupling parameter. The dynamical roles of relaxation oscillations and semiconductor features are analysed by using simple laser models that can be numerically integrated by using Matlab.

In the second part of the project, we remove the losses due to the spontaneous emission of photons and obtain equations that are (surprisingly) reversible in time. The research will focus on the coexistence of conservative and dissipative dynamics [1] that can lead to unexpected oscillations of the coupled laser output. Coupled lasers, laser arrays and laser networks [2] find natural applications in optical communications and in the processing of optical information.

#### **Key Reference (if applicable):**

[1] D. H. Henderson, PhD Thesis "Reversibility and intensity dependent dissipations in lasers" (University of Strathclyde, 2000)

[2] M. Nixon et al., "Controlling synchronization in large laser networks", Phys. Rev. Lett. **108**, 214101 (2012)

Ratio of effort: Exp/Theo/Comp Exp: 10 %

Theo: 40 % Comp: 50 %

**Suitability:** MPhys, BSc (including Maths Physics)

**Additional comments:** The "experimental" part is related to the understanding of experimental results and their comparison with numerical simulations.

# Simulations of Spin-Polarized Vertical-Cavity Surface-Emitting Lasers

Project Supervisors: (1) Prof. Gian-Luca Oppo, (2) Prof. Thorsten Ackemann

#### **Project Description:**

Spin-polarized vertical-cavity surface-emitting lasers (known as VCSELs) offer the exciting prospect of output polarization control through the injection of spin-polarized electrons. Such capabilities could lead to many new applications in the field of spectroscopy, communications and information processing. In this project we simulate the rate equations that describe the right- and left-circularly polarized complex fields and the carrier densities, as originally introduced in [1], to detect and describe the instabilities leading to self-sustained oscillations [2]. The numerical integration is made via MATLAB while the output is characterized by power and optical spectra. We look at the description of Vertical External Cavity devices, bifurcation diagrams, high frequency oscillations and possible transitions to chaotic motion for spin-polarized lasers. The effects of an injected signal and modulations of losses or cavity parameters are also investigated.

## **Key Reference (if applicable):**

[1] G. P. Puccioni, M. V. Tratnik, J. E. Sipe and G.-L. Oppo, "Low instability threshold in a laser operating in both states of polarization" Optics Letters **12**, 242 (1987)

[2] R. Al-Seyab, D. Alexandropoulos, I. D. Henning, and M. J. Adams, "Instabilities in Spin-Polarized Vertical-Cavity Surface-Emitting Lasers" IEEE Photonics Journal **3**, 799 (2011)

Ratio of effort: Exp/Theo/Comp Exp: 10 %

Theo: 40 % Comp: 50 %

Suitability: MPhys, BSc

**Additional comments:** Good performance in the course PH254 Computational Physics is recommended. The "experimental" part is related to the understanding of experimental results and their comparison with numerical simulations.

**Plasmas Division** 

# Non-linear Optics in Plasma: Raman Amplification and Frequency Mixing

Project Supervisors: (1) Prof. Dino Jaroszynski, (2) Dr Bernhard Ersfeld

#### **Project Description:**

This project offers the opportunity to investigate, both theoretically and numerically, non-linear interactions between (transverse) electromagnetic waves through a (longitudinal) plasma wave. It has been suggested to use such a process, stimulated Raman scattering, to amplify a seed pulse by extracting energy from an intense pump pulse to provide a new type of light amplifier to reach petawatts, exawatts and beyond. Plasma as a non-linear optical medium for intense laser pulses has additional interest when optical pulses are sufficiently intense to drive electrons (and holes or positrons) to relativistic energies, and thus to generate astrophysical conditions in the laboratory.

The investigation may build on an existing code for the hydrodynamic simulation of plasma taking into account a variable number of carrier species, such as electron-positron plasmas, and electrons and ions, or holes in the case of a semiconductor plasma.

**Reference:** William L. Kruer: The physics of laser plasma interactions, Addison-Wesley, Redwood City, Calif. c1988. Main Library: D 530.44 KRU (or other textbooks on laser-plasma interaction)

Ratio of Experiment/Theory/Computation: Exp: 0 %

Theo: 50 % Comp: 50 %

Suitable for: MPhys, BSc (Maths Physics)

**Additional Comments:** Knowledge in the following areas would be advantageous: wave propagation, Fourier theory; computer programming (C or similar). Anyone interested in taking up this project should contact the supervisors beforehand.

**Safety Training Requirements:** Contact the project Supervisor for further advice

# **Electron Beam Transport and Diagnostics**

# Project Supervisors: (1) Prof. Dino Jaroszynski, (2) Dr Enrico Brunetti

#### **Project Description:**

Laser-driven particle accelerators are compact sources of high quality electron beams with potential applications to fields such as medicine, biology and material science. Since many applications require the transport and focusing of a beam over long distances, a good quality transport system is essential. This project consists of the theoretical study of the transport of an electron beam through magnetic devices, with particular emphasis on properties such as transverse emittance and bunch length.

**Reference:** Wiedemann, Particle Accelerator Physics, Springer, 2007 Jackson, Classical Electrodynamics, Wiley, 1999 Esarey, Schroeder and Leemans, Physics of laser-driven plasma-based electron accelerators, Rev. Mod. Phys. 81, 1229–1285 (2009)

Ratio of Experiment/Theory/Computation: Exp: 0 %

Theo: 50 % Comp: 50 %

**Suitable for:** MPhys, BSc (Maths Physics)

**Additional Comments:** Knowledge in the following areas would be advantageous: wave propagation, Fourier theory; computer programming (C or similar). Anyone interested in taking up this project should contact the supervisors beforehand.

Safety Training Requirements: Contact the project Supervisor for further advice

# **Induced Relativistic Optical Transparency in Intense Laser-Solid Interactions**

Project Supervisors: (1): Prof. Paul McKenna, (2) Dr Ross Gray

#### **Project Description:**

By focusing petawatt-scale pulses of laser light to intensities exceeding  $10^{20}$  Wcm<sup>-2</sup>, novel states of matter are created, involving highly relativistic plasma. The propagation of light in such plasma results in nonlinear effects analogous to those studied with conventional nonlinear optics, including for example self-focusing, self-modulation and harmonic generation. Laser light cannot normally propagate above a critical density at which the oscillating plasma frequency is equal to the laser frequency. However, at ultra-high intensities the quiver motion of the electrons in the laser field becomes relativistic and electron mass is increased by the Lorentz factor,  $\gamma$ . As a consequence of the increased relativistic inertia of the electrons the plasma frequency changes, increasing the critical density, leading to induced relativistic optical transparency, so that light can propagate through what would otherwise be over-dense or opaque plasma.

The objective of this project is to investigate the onset of relativistic optical transparency in dense plasmas irradiated by ultra-intense laser pulses. This involves simulating the response of the plasma electrons and ions to the fields created at the focus of the laser pulse, using a particle-in-cell code running on a high performance computer.

Ratio of effort: Exp/Theo/Comp Exp: %

Theo: 20% Comp: 80%

**Suitability:** BSc, BSc (Phys with Teaching), BSc (Maths Physics)

# **Design Study on Plasma Optics**

Project Supervisors: (1) Prof. Paul McKenna, (2): Dr Ross Gray

#### **Project Description:**

The conventional approach to focusing light, based on the use of solid state optical media, has not fundamentally changed over the centuries, but is rapidly becoming a key limiting factor for the further development of ultraintense laser science. The main reason for this is that there is a limit to the energy density which solid state optical media can withstand before it is damaged. The traditional way to circumvent this is to increase the size of the focusing optic as the laser energy is increased, so that the overall energy density is below the critical value. However, the optics used on the highest power lasers are now more than a meter in diameter and are very expensive. Radical new approaches are required for the production of compact high intensity laser drivers for application.

The project aims to explore the feasibility of developing new types of optical systems based on ultrafast plasma processes —plasma optics. Due to their ability to sustain extremely large amplitude electromagnetic fields, plasma optical components are inherently compact, and the ultrafast evolution of the optical properties of laser-excited plasma enables other properties of the laser pulse to be tailored. The project involves designing new plasma optical components using optical design programmes and plasma simulation codes.

Ratio of effort: Exp/Theo/Comp Exp: %

Theo: 20 % Comp: 80 %

**Suitability:** BSc, BSc (Phys with Teaching), BSc (Maths Physics)

# Modelling Laser-driven Plasma Expansion and Ion Acceleration Dynamics

Project Supervisors: (1) Prof. Paul McKenna, (2) Dr. Ross Gray

#### **Project Description:**

The interaction of intense laser pulses with matter is opening up new frontiers in physics via the production of extreme pressures, temperatures and intense electric and magnetic fields. This is leading to the use of high power laser radiation for exploring the properties of hot dense matter, the production of high energy particles and radiation, and the development of schemes to generate energy by inertial confinement fusion. The possibility of using high power lasers to generate high-quality beams of energetic ions is attracting global interest. In particular, laser-based ion acceleration schemes may lead to compact and relatively low-cost sources which can be used in science, medicine and industry.

The project involves modelling the acceleration of ions in electrostatic fields formed on the surface of thin foil solid targets which are irradiated by ultra-intense laser pulses. Specifically, it involves writing a code using Matlab to model the dynamics of the evolving electrostatic field and how that maps into the spatial-intensity profile of the beam of ions accelerated. The code will be applied to analysis existing experimental data obtained using a number of high power laser facilities. It will provide the student with a background in the physics of high power laser-based sources of ions, diagnostic techniques and in simulation and modelling.

**Key Reference:** 

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 20% Comp: 80%

Suitability: BSc, BSc Maths and Physics, BSc Physics with Teaching

Additional comments:

# Theoretical and Numerical Studies of Laser Pulse Compression in Underdense Plasma

Project Supervisors: (1) Prof. Zheng-Ming Sheng, (2) Prof. Dino Jaroszynski

### **Project Description:**

Plasma as the fourth state of matter is pervasive in space, laboratory, and also in our life. It is formed when bounded electrons are released from atoms (such as by high electric fields of a laser pulse) to become free electrons so that the system is made of free electrons and ions. The plasma as a medium exhibits distinct electric and magnetic properties, different from those in normal gas and solid targets. Recently with the development of chirped pulse amplification (CPA) technology, one can produce ultrashort and high intensity laser pulses. Such laser pulses can find wide applications including charged particle acceleration, high power X-ray radiation, advanced laser fusion, and the creation of high energy density matter etc.

Currently, typical high power laser pulse duration is about 40-50fs. For some applications, one needs to the laser pulse duration can be further reduced to less than 30fs. It is found that the plasma as a nonlinear medium can be used to compress the high intensity laser pulse. The main task of this project is to find suitable plasma parameters to compress the laser pulse duration.

### **Key Reference:**

1. H. Y. Wang et al., Phys. Rev. Lett. 107, 265002 (2011).

2. O. Shorokhov et al., Phys. Rev. Lett. 91, 265002 (2003).

3. Z. M. Sheng et al., Phys. Rev. E 62, 7258 (2000).

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 30% Comp: 70%

**Suitability:** MPhys, BSc, BSc Maths and Physics, BSc Physics with Teaching

**Additional comments:** For different degree levels, the project will be carried out at different depths such as one-dimensional model, two-dimensional model, for laser pulses at different laser intensities, etc.

**Safety Training Requirements: No** 

# Nonlinear Propagation of Extreme Intense Laser Beams in Plasma

Project Supervisors: (1) Prof. Zheng-Ming Sheng, (2) TBC

### **Project Description:**

Plasma as the fourth state of matter is pervasive in space, laboratory, and also in our life. It is formed when bounded electrons are released from atoms (such as by high electric fields of a laser pulse) to become free electrons so that the system is made of free electrons and ions. The plasma as a medium exhibits distinct electric and magnetic properties, different from those in normal gas and solid targets. Recently with the development of chirped pulse amplification (CPA) technology, one can produce ultrashort and high intensity laser pulses. Such laser pulses can find wide applications including charged particle acceleration, high power X-ray radiation, advanced laser fusion, and the creation of high energy density matter etc.

Currently, the Extreme Light Infrastructure (ELI) is under construction in Europe (<a href="http://www.eli-laser.eu/">http://www.eli-laser.eu/</a>). Future ELI laser beams may reach peak power of 10-100PW (1PW=10^15 W). For a number of applications, it is interesting and necessary to investigate how such laser beams propagate in plasma. It is expected that nonlinear effects such as the relativistic electron motion and ponderomotive force play key roles for the laser propagation. In some cases, even the radiation reaction can play a role. The main task of this project is to investigate theoretically and numerically how such lasers will propagate based upon the envelop equation for laser beam derived with the paraxial approximation.

## **Key References:**

- 1. W.-M. Wang, Z.-M. Sheng et al., Appl. Phys. Lett. 101, 184104 (2012).
- 2. Z.-M. Sheng et al., Phys. Rev. E 64, 066409 (2001).
- 3. M. Chen et al., Plasma Phys. Control. Fusion 53, 014004 (2011).

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 20% Comp: 80%

**Suitability:** MPhys

**Additional comments:** I have a model and code developed. The student is required to extend this work. It is preferable that the student is interested in programming.

**Safety Training Requirements: No** 

# Beam-driven Plasma Wakefield Acceleration (PWFA)

# Project Supervisors: (1) Prof. Bernhard Hidding, (2) Prof. Dino Jaroszynski

# **Project Description:**

Electron beams can drive plasma waves for generation and acceleration of highest brightness electron beams, which is strongly desired for advanced free-electron lasers. Suitable electron beam drivers can be produced by conventional accelerators such as SLAC as well as by laser wakefield acceleration. PWFA is a highly trending field and will be studied in by means of particle-in-cell simulations as well as in experiments in which the electron bunch output from laser-plasma-accelerators in Strathclyde will be used for the first time for PWFA. One special additional feature is the development of the underdense photocathode (aka Trojan horse) concept [1-2].

**Key Reference (if applicable): [1]** B. Hidding, G. Pretzler, J.B. Rosenzweig, T. Königstein, D. Schiller, D.L. Bruhwiler, *Ultracold Electron Bunch Generation via Plasma Photocathode Emission and Acceleration in a Beam-driven Plasma Blowout*, Physical Review Letters 108, 035001, 2012 (4 pages) [2] *Hybrid modeling of relativistic underdense plasma photocathode injectors* 

Y. Xi, B. Hidding, D. Bruhwiler, G. Pretzler, and J. B. Rosenzweig, PRSTAB 16, Issue 3, 031303 (2013)

Ratio of effort: Exp/Theo/Comp Exp: 40%

Theo: 20% Comp: 40%

**Suitability:** MPhys, BSc, BSc (Phys with Teaching), BSc (Maths Physics)

**Additional comments:** Knowledge in laser and plasma and accelerator physics is helpful but not mandatory. Anyone interested in taking up this project should contact the supervisors beforehand.

Safety Training Requirements: Contact the project supervisor for further advice

# **Excitation of Heavy Atomic Species for ITER**

Project Supervisors: (1) Prof. Nigel Badnell, (2) Prof. Bob Bingham (tbc)

# **Project Description:**

The development of the ITER device for magnetic fusion requires the use of much heavier elements (Kr, Xe, W etc) than have traditionally been used, such as at the JET device.

Consequently, spectroscopic diagnostic modelling at ITER, which is already being simulated, requires atomic data where relativistic effects are likely much larger than have been seen before. The goal of the project is to assess the degree of importance of relativistic effects of relevance to ITER diagnostics. This will entail computational calculations of atomic data with varying degrees of treatments of relativistic effects viz. non-relativistic vs relativistic wavefunctions, the importance of the Breit interaction and the validity of its Pauli approximation at `low'-charge.

Key Reference (if applicable): <a href="http://www.iter.org/">http://www.iter.org/</a>

Ratio of Experiment/Theory/Computation: Exp: 0 %

Theo: 30 % Comp: 70 %

Suitable for: MPhys

**Additional Comments:** Familiarity with Unix (e.g. Linux) working environment and good computing skills in general.

**Safety Training Requirements:** 

# Stochastic Particle Heating of Charged Particles by Plasma Waves

Project Supervisors: (1) Dr Bengt Eliasson, (2) Dr Kevin Ronald

## **Project Description:**

Plasmas are ubiquitous in space and laboratory. The Earth is surrounded by a plasma layer, the so-called ionosphere, which shields us from radiation and energetic particles from the sun, and in the laboratory, plasmas are artificially created and studied with application to magnetic confinement fusion and basic research. A plasma is an ionised gas in which there are free electrons and ions so that the gas is electrically conducting. The Earth's ionosphere is magnetized by the geomagnetic field, and in the laboratory, an external magnetic field is used to confine the plasma and prevent it from escaping to the walls. The acceleration of charged particles by electromagnetic waves can lead to chaotic motion of the particles and a rapid heating of the magnetised plasma due to the complicated motion of the particles. This is important for heating of particles in the laboratory, in magnetic confinement fusion devices, in the solar corona, in the Earth's ionosphere, etc., where collisions between particles are relatively rare. Stochastic heating is therefore different from Ohmic heating which is due to collisions between particles.

The project involves at building a numerical model for stochastic heating of charged particles (electrons and/or ions) in magnetized plasmas by using test-particle simulations, and to use the numerical model to study some different cases where stochastic heating takes place. A theoretical derivation and understanding of the mathematical models is also part of the project.

**Key Reference:** J. M. McChesney, R. A. Stern, and P. M. Bellan (1987) Observation of fast stochastic ion heating by drift waves, Phys. Rev. Lett. 59, 1436-1439.

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 50% Comp: 50%

**Suitability:** MPhys, BSc, BSc Maths and Physics

**Additional comments:** Experience in simulations using Matlab (or any other programming language) and good theoretical skills are beneficial.

**Safety Training Requirements:** 

# Numerical Modelling and Design of a High Power Magnetron

# Project Supervisors: (1) Dr Alan Young, (2) Prof. Adrian Cross

# **Project Description:**

Magnetrons are one of the most efficient and widely used high power microwave sources in existence today. Reliable magnetron operation is one of the main reasons for their use in numerous applications such as marine radar, radio frequency (RF) acceleration in medical LINACS for radiotherapy treatment of cancer, microwave processing and heating of materials.

The theory and design of a high power magnetron used in a medical LINAC will be studied. Numerical modelling of the magnetron will be carried out using CST Particle Studio. As the formation of a rotating electron space charge limited beam occurs in the same physical space as the RF interaction region the full capability of an advanced computer graphics processing unit will be used to carry out the simulations. The goal of the project will be to develop a numerical model that can be used to predict the output power and efficiency of the magnetron as compared to its existing experimental data.

### **Key References:**

[1] A.F. Harvey, "Microwave Engineering", Academic Press, London and New York, 1963.

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 40% Comp: 60%

**Suitability:** BSc, BSc Maths and Physics

### **Additional comments:**

**Safety Training Requirements:** High voltages will <u>not</u> be used and X-ray emission will <u>not</u> be generated during this project.

# Design of a Brewster Window for a W-band Gyro-TWA

# Project Supervisors: (1) Dr Liang Zhang, (2) Prof. Adrian Cross

### **Project Description:**

A W-band gyrotron-travelling wave amplifier (gyro-TWA) based on a helically corrugated waveguide and a cusp electron gun is currently being studied. It is predicted to achieve an output power of 5 kW over a wide frequency band of 90 - 100 GHz. For an amplifier the microwave window, which separates the high vacuum side from the atmospheric pressure outside must couple in or out the microwave power with minimum absorption or reflection, and is one of the critical components for the successful operation of the gyro-TWA.

In this project, a Brewster-type microwave window will be studied using analytical theory. Numerical simulations Brewster-type microwave window will be carried out using CST Microwave Studio. A corrugated waveguide that maintains the Gaussian-like HE mode required for the Brewster window will also be designed and simulated. The design goals of the Brewster window are 10% bandwidth at a centre frequency of 95 GHz, small insertion loss and a reflection of less than -20 dB for the operating band. If the design meets the requirement, the Brewster window will be manufactured and measured using a Vector Network Analyser (VNA).

### **Key References:**

[1] Wenlong He, Craig R. Donaldson, Liang Zhang, Kevin Ronald, Paul McElhinney and Adrian W. Cross, "High Power Wideband Gyrotron Backward Wave Oscillator Operating towards the Terahertz Region", Physical Review Letters, 110(16):165101, 04, 2013.

[2] Paul McElhinney, Craig R. Donaldson, Liang Zhang and Wenlong He, "A High Directivity Broadband Corrugated Horn for W-band Gyro-devices", IEEE Transactions on Antennas and Propagation, vol. 61, no. 3, pp. 1453-1456, 2013.

Ratio of effort: Exp/Theo/Comp Exp: 20%
Theo: 30%
Comp: 50%

**Suitability:** MPhys, BSc, BSc Maths and Physics

### Additional comments:

**Safety Training Requirements:** High voltages will <u>not</u> be used and X-ray emission will <u>not</u> be generated during this project although a risk assessment will need to be completed in semester 1.

# Monte Carlo Simulation and Cooling Performance of the MICE Step V Laboratory Experiment.

Project Supervisors: (1) Dr David Speirs, (2) Dr Kevin Ronald

### **Project Description:**

A Neutrino Factory based on a muon storage ring represents the ultimate tool for the study of neutrino oscillations, including the potential discovery of leptonic CP violation. It is also the first step towards the construction of a  $\mu+\mu-$  collider. Ionisation cooling of muons can make a significant contribution to both the performance (up to a factor of 10 in neutrino intensity) and cost (as much as 20%) of a Neutrino Factory. This potential benefit has motivated the undertaking and construction of the Muon Ionisation Cooling Experiment (MICE), a significant undertaking that has various key stages in its physical implementation. There are various potential lattice configurations currently under consideration for MICE Step V - the final operating configuration for the experiment. Simulating and evaluating these potential configurations is currently a critical activity in order to implement a successful MICE Step V experiment. The aim of this project is therefore to conduct a variety of simulations using the MICE Analysis User Software (MAUS), a Monte Carlo Simulation Tool which predicts the trajectories of the muons through a complex system of magnetic fields, solid beamline objects and accelerating cavities, to determine and evaluate the most suitable Step V lattice configurations and operating conditions, and to define the performance requirements of key detectors to ensure a successful MICE experiment and first practical demonstration of ionisation cooling.

**Key Reference:** Adams D. et al, 2013, 'Characterisation of the muon beams for the Muon Ionisation Cooling Experiment' Euro. Phys. J. C, **73**, art. 2582

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 30% Comp: 70%

**Suitability:** MPhys, BSc, BSc Maths and Physics, BSc Physics with Teaching

**Additional comments:** 

**Safety Training Requirements:** 

# Design and Measurement of a Mode Converter for a Microwave Amplifier

Project Supervisors: (1) Dr Wenlong He, (2) Dr Craig Donaldson

### **Project Description:**

A microwave amplifier in the form of a gyrotron traveling wave amplifier is being studied at the University of Strathclyde. The amplifier uses the interaction between a rotating electron beam and a low power microwave signal to amplify the microwaves to high power over a wide bandwidth. In order to have the correct interaction a low power microwave signal needs to go through a mode converter to change from a  $TE_{1.1}$  mode to a  $TE_{3.1}$  mode.

In this project, a mode converter will be studied using analytical theory. Numerical simulations will be carried out using CST Microwave Studio. This converter is a four-fold helical corrugated waveguide. Initially this will be studied and measured using a vector network analyser (VNA), at X-band frequencies ~9 GHz.

In year 2 of the project the converter will be scaled down in size to operate at a much higher frequency in the W-band, at  $^{\sim}$  94 GHz. In both applications the converter will have to operate over the amplifiers bandwidth range of 10GHz and have a high conversion efficiency whilst maintaining a low reflection coefficient.

**Key Reference:** He W., Donaldson C.R, Zhang L., Ronald K., McElhinney P., and Cross A.W., "High power wideband gyrotron backward wave oscillator towards the terahertz region", Phys. Rev. Letts, 110, art 165101, (2013).

Ratio of effort: Exp/Theo/Comp Exp: 25%

Theo: 25% Comp: 50%

Suitability: MPhys

### **Additional comments:**

**Safety Training Requirements:** High voltages and X-ray emission will <u>not</u> be required for this project although a risk assessment will need to be completed in semester 1.

**Institute of Photonics** 

# **Modelling Non-linear Processes in Micro-waveguides**

# Project Supervisor (1) Dr Michael Strain, (2) Dr Nicolas Laurand

# **Project Description**

Waveguides with sub-micron cross-sectional dimensions have proven extremely successful in non-linear optical applications. By using materials with high refractive index, such as silicon, light can be confined into ultra-small volumes, producing extremely high local field intensities. If these materials also exhibit an optical non-linearity, i.e. their susceptibility\refractive index is a function of the strength of the optical field, then a wide array of devices can be designed. For example, ultra-fast photonic switches can be created that are triggered using optical pulses (i.e. without the need for electronics) with potential applications in optical signal processing. Non-linear processes can also create new wavelengths of light in a device, for example allowing a signal input at  $\lambda_1$  to be broadcast on a wide range of new wavelengths, simply by propagating through a non-linear device. Finally, these devices can take a single laser wavelength input and, through self-phase modulation, generate a supercontinuum of light.

The effects of dispersion in non-linear waveguides are critical in the design of these devices. The refractive index as a function wavelength of nanowire waveguides exhibits a strong dependence on the waveguide geometry. The dispersion induced by the waveguide in turn induces variation in the non-linear optical processes in the waveguide. In order to achieve efficient operation, a balance must be achieved between increasing the field intensity by reducing the waveguide cross sectional area and finding the optimal waveguide dispersion regime.

In this project the student will use numerical tools to model the dispersive behaviour of nanowire waveguides in a variety of materials. This analysis will then underpin further calculation of the non-linear effects in nanowire waveguides, with particular reference to self-phase modulation and four wave mixing processes. The student will write customised simulation codes to probe the behaviour of these waveguides and compare their results with experimental demonstrations.

### **Key Reference (if applicable):**

- 1. Q. Lin, O. J. Painter, and G. P. Agrawal, "Nonlinear optical phenomena in silicon waveguides: modeling and applications.," Opt. Express, vol. 15, no. 25, pp. 16604–44, Dec. 2007.
- 2. J. Leuthold, C. Koos, & W. Freude, "Nonlinear silicon photonics," Nature Photonics, 4(8), 535–544, 2010.
- 3. A.C. Turner, M.A. Foster, A.L. Gaeta, M. Lipson, "Ultra-low power parametric frequency conversion in a silicon microring resonator," Optics express, 16, (7), p. 4881-7, 2008.

Ratio of effort: Exp/Theo/Comp Exp: 0%

Theo: 50% Comp: 50%

Suitability: MPhys, BSc

Additional comments: Some previous experience of Matlab would be beneficial but not essential.

**Safety Training Requirements: NA** 

# **Allocated Projects (Fifth Year students)**

Project Name	Supervisors	Student Name
Spectroscopic Studies of Pheomelanin: Spectra, Kinetics, Modulators	Jens Sutter, David Birch	Junaid Ahmad
Exotic quantum operations with light	John Jeffers, Daniel Oi	Liviu Chirondojan
Optical Properties of Nanoparticles	Yu Chen, Olaf Rolinski	Chloe Chung
Highly efficient frequency up-conversion in Rb vapour	Aidan Arnold, Erling Riis	Craig Colquhoun
The theory of X-ray Free electron Lasers	Brian McNeil, Gordon Robb	Sean Davies
Holographic Atom Traps	Stefan Kuhr, Elmar Haller	Charelle Dunbar- Dawe
Effects of electron irradiation on photoluminescence spectra of thin film Cu(InGa)Se2	Rob Martin, Michael Yakushev	Rachel Elvin
Electroluminescence spectroscopy and electrical characterisation of light-emitting diodes	Rob Martin, Paul Edwards	Catherine Freeke
Radiotherapy using Beams from Laser-plasma Accelerators	Dino Jaroszynski, Silvia Cipiccia	Gregor Garbutt
BEC-light interactions	Gordon Robb, Gian-Luca Oppo	Kristofer Gray
Optical forces on nanoparticles	Ben Hourahine, Francesco Papoff, Gordon Robb	Robert Harris
Simulation of electromagnetic waves in magnetized plasmas	Bengt Eliasson, Kevin Ronald, David Speirs	Timothy Heelis
The Physics of DNA	Neil Hunt, Glenn Burley	Stephen Howorth
Radiotherapy using Beams from Laser-plasma Accelerators	Dino Jaroszynski, Silvia Cipiccia, Xue Yanh	Matthew Lebessis
Laser-Wakefield Plasma Accelerated electron optimization for Very High Energy Electron (VHEE) cancer treatment	Dino Jaroszynski, Silvia Cipiccia	Alexander MacDonald
Radiation Reaction	Dino Jaroszynski, Adam Noble	Alexander MacLeod
High energy ion acceleration in intense laser- plasma interactions	Paul McKenna, Ross Gray	John McCreadie
Eu-doped GaN	Kevin O'Donnell, Rob Martin	Ivan Morgan
Capillary Discharge Waveguides for Laser- Plasma Interactions	Dino Jaroszynski, Mark Wiggins	Lewis Reid
The scientific applications of X-ray Free Electron Lasers	Brian McNeil, Gordon Robb	James Simpson
Optical Second Harmonic Generation in Urea	Tom Han, Nigel Langford	Neil Stevenson
Nanoparticle Metrology	David Birch, Jens Sutter	Hazel Stewart
Testing for gravitational coupling to Entropy	Nick Lockerbie, Tom Han	Peter Tinning

# **Appendices**

# Safety induction training record for Undergraduate students undertaking project work

This form **MUST** be completed by student and supervisor and returned **before** student enters a laboratory and by 28th November 2014 at the **latest**.

1)	I have read and understood the 'Local rules for the Safe Use of
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Please return this completed form to Students Office, JA 8.31

# **Project allocation request form 2014/15**

(To be returned by the student to Students Office JA 8.31 by 4pm 03/10/14)

Student Name:	Student Number:	
Project title:		
Supervisor's signature:	This project has been discussed by us, and we have agreed that it is	
Supervisor's name:	appropriate for the student to undertake the work.	
Student's signature:		
Preference:	For student to choose on completion of the form	
Project title:		
Supervisor's signature:	This project has been discussed by us, and we have agreed that it is	
Supervisor's name:	appropriate for the student to undertake the work.	
Student's signature:		
Preference:	For student to choose on completion of the form	
	-	
Project title:		
Supervisor's signature:	This project has been discussed by us, and we have agreed that it is	
Supervisor's name:	appropriate for the student to undertake the work.	
Student's signature:		
Preference:	For student to choose on	

Note: where several allocation request forms are submitted for the same project, I will choose the successful student by lot.

Projects allocated will be announced by Timothy Briggs on Wednesday the 8<sup>th</sup> October 2014 – Kevin O'Donnell

## **Project Timetables**

#### PH450

Taken in 4<sup>th</sup> year by MPhys and BSc Physics.

Optional for BSc Physics with Teaching and BSc Mathematics and Physics students

**22<sup>nd</sup> September 2014** Project booklet to students

Students will receive project handbook with project request page.

22<sup>nd</sup> September –3<sup>rd</sup> October 2014 Students choose projects

Students should visit supervisors and draw up a shortlist of 3 potential projects in order of preference from 1 to 3. Each project request must be signed and dated by both the student and the supervisor and submitted to the student office, JA8.31.

**4pm 3<sup>rd</sup> October 2014** Deadline for submission of Project choice form to JA8.31

8<sup>th</sup> October 2014 Official start of Projects

Project allocations announced at 12 noon through Myplace. Students who have been unsuccessful in getting their choice of project will receive an updated booklet for a second round.

27<sup>th</sup> October 2014 Literature review complete

Students submit literature survey and a risk assessment for project. The literature review will usually take the form of the Final Report's introductory chapter.

**28**<sup>th</sup> **November 2014** Completed safety form to be returned to JA 8.31 by this date

**30**<sup>th</sup> January **2015** Progress report with aims of project to be returned by students to JA 8.31

by this date

**25**<sup>th</sup> March & 1<sup>st</sup> April 2015 Project Talks 1-5 pm in parallel Sessions

Each student will be given a 15-minute slot. The expectation is that students will talk about their project for 10 minutes and then be questioned by the audience for 5 minutes.

**20<sup>th</sup> April 2015** Project reports submitted

Project reports to be submitted as Word or PDF format through MyPlace and then passed through Turnitin for plagiarism detection.

In preparing the report, please be aware that supervisors can advise on up to 10 pages of material, to help with the style of writing and content, but not to correct physics.

Week beginning 5<sup>th</sup> May 2015 Viva week

Each viva will be about 35 minutes long, with 5 minutes for the student to outline their project work and 30 minutes of questions about project content.

# **Project Information for Continuing 5<sup>th</sup> Year Students**

#### PH 550

Taken in 5<sup>th</sup> year by MPhys Physics students. The expectation is that students will continue with the project started in 4<sup>th</sup> year.

Week beginning 30<sup>th</sup> September Meeting with supervisor during Week 1

Projects should be underway by 8<sup>th</sup> October

**7<sup>th</sup> November 2014** Progress report to be returned by students to JA 8.31 by this date

**10**<sup>th</sup> **December 2014** Project Talks 1-5 pm in parallel sessions

Each student will be given a 15-minute slot. The expectation is that students will talk about their project for 10 minutes and then be questioned by the audience for 5 minutes.

23<sup>rd</sup> January 2015 Project papers submitted

Project papers to be submitted as PDF format through MyPlace and then passed through Turnitin for plagiarism detection.

Week beginning 2<sup>nd</sup> February 2015 Vivas

Each viva will be about 35 minutes long, with 5 minutes for the student to outline their project work and 30 minutes of questions about project content.

#### Plagiarism

Plagiarism most commonly involves the passing off of another person's work as your own and is regarded as a form of academic dishonesty. Plagiarism more often than not involves the copying of another person's work, be it a figure, text, experimental data or homework for example and not acknowledging the source of the work. Plagiarism can be avoided by suitable referencing.

For more details on plagiarism please see the University Handbook and follow this link <a href="http://www.strath.ac.uk/media/ps/cs/gmap/plagiarism/plagiarism student booklet.pdf">http://www.strath.ac.uk/media/ps/cs/gmap/plagiarism/plagiarism student booklet.pdf</a> for guidelines on plagiarism. If you are unsure of any aspect of this, please contact the department. The department will make extensive use of software capable of detecting plagiarism. The Department will use the anti-plagiarism software Turnitin (<a href="https://turnitin.com/static/index.php">https://turnitin.com/static/index.php</a>) to check for plagiarism. Any student caught plagiarising another person's work may be reported to the University Disciplinary committee.

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