School of Physics Senior Sophister Projects 2025-26
Theoretical Physics

August 8, 2025

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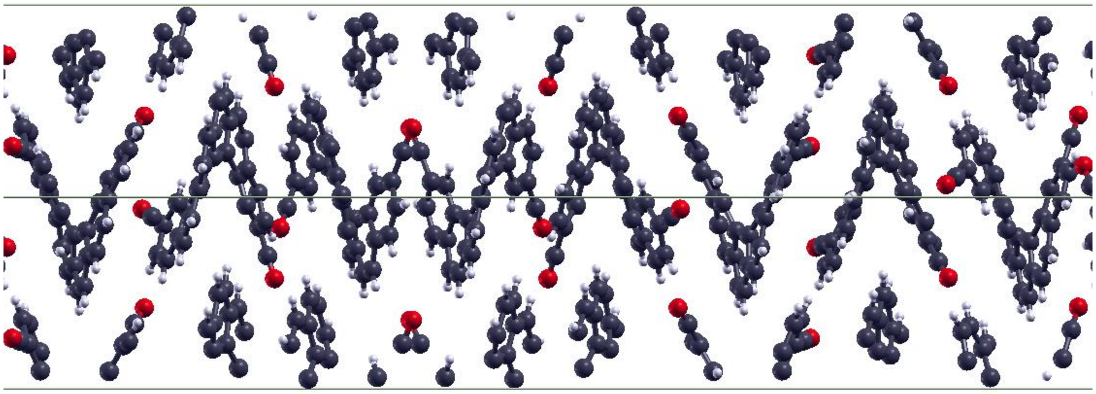
Circular dichroism in helicene chiral molecules

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

Circular dichroism (CD) is a property of matter in which optical properties depend on the handedness of circularly polarised light incident on the material. For non-zero CD properties to exist, the material concerned must be chiral. That is, the material must be left- or right-handed. Many naturally occurring organic molecules exist as pairs of *enantiomers*, with the left-handed enantiomer usually predominating in nature.

Helicenes are chiral acene molecules in which a sequence of fused benzene rings are arranged in a nearly full circle. Steric repulsion effects between the ends of these molecules mean that the molecular structure is a short helix, with an inherent handedness. Recent work at Imperial College London has (which featured in a recent School Seminar by Prof. Jessica Wade) demonstrated that addition of helicenes to poly-fluorene results in circularly polarised luminescence by an organic light emitting diode (OLED).

In this project you will calculate the CD spectrum of helicene molecules using time-dependent density functional theory with the aim of understanding how CD arises in helicene molecules. Which quantum states are involved in CD and what are the strengths of optical transitions which result in CD? This project will afford you the opportunity to learn about molecular quantum mechanics and computational physics.



Aza-helicene crystal structure

Highly Efficient Inverted Circularly Polarized Organic Light-Emitting Diodes, L. Wan, J. Wade, X. Shi, S. Xu, M. J. Fuchter and A. J. Campbell, ACS Appl. Mater. Interfaces, 12, 39471 (2020).

Trinity College Dublin
The University of Dublin

Molecular Thermodynamics of Xylopyranose Structural Motifs: A Quantum Chemistry Approach

Advisor: Prof. Stephen Dooley (P.I.)

Co-advisor: Ph.D. Leandro Ayarde Henríquez (P.R.)

Abstract The unrenewable character of fossil fuels and the increasing social demands have led academia and industrial sectors to explore alternative sources from which energy can be drawn and used. In this context, biomass degradation via pyrolysis yields many valuable bio-products (including fuels), supporting a bio and circular economy. However, the molecular mechanism of the depolymerization processes is far from clear, hindering the development of pyrolysis technologies and the use of bio-products in everyday life. Thus, this proposal aims to gauge high-performance computing (HPC) systems for automatedly exploring the potential energy surfaces (PESs) of xylopyranose motifs under pyrolysis conditions in combination with sophisticated quantum chemistry methodologies, including composite model chemistry methods (e.g., CBS-QB3 and G4) and domain-based local pair natural orbital (DLPNO). This strategic approach is crucial to understanding electron reorganizations along a reaction pathway that underpin both the reaction mechanism and thermos-kinetics and will ultimately contribute to the faster deployment of sustainable bio-products at a commercial scale. These calculations comprise the first systematic study regarding biomass thermal decomposition.

Structure and visualisation of quantum instruments in finite dimensions

Project aim and abstract. The aim of this project is to characterise and visualise the structure and optimisation landscape of quantum instruments, with the goal of understanding their geometric, topological, and operational properties.

Quantum instruments are hybrid quantum/classical objects that describe both the classical outcomes of a measurement and the corresponding updates to a quantum state. They generalise the notion of postive operator valued measures (POVMs) by encoding outcome probabilities together with a post-measurement state update.

This project investigates the geometric and algebraic structure of the space of quantum instruments in finite-dimensional Hilbert spaces. We focus on the qubit and qutrit cases, in order to find a meaningful visualization and to allow tractable numerical exploration. The project aims to characterise features such as convexity, extremal points, and decompositions. The student is expected to build numerical simulations and visual representations of these structures, which offer physical insights. This project is well-suited for a mathematically inclined student with an interest in quantum information, linear algebra, and optimisation. Some elementary references on quantum instruments can be found here: [1–4].

References

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Quantum Information Theory Group

Project proposal: Local thermality from global athermality

Thermodynamics exhibits a profound connection with information theory. The erasure of information incurs an energetic cost [1], while, conversely, stored information can be exploited to extract useful work [2]. In the quantum regime, correlations—particularly quantum correlations such as entanglement—serve as fundamental resources that enable tasks impossible or inefficient in classical settings. Investigating the thermodynamic aspects of these correlations offers valuable insights into how information is physically distributed and processed in quantum systems, as well as the associated energetic costs.

Pioneering research in this direction has demonstrated thermodynamic advantages arising from the presence of correlations [3-5]. Building on these developments, this project proposes to employ and extend existing methods [6] to characterize the role of classical and quantum correlations in local thermal states. These are states that appear to be in thermal equilibrium from the perspective of each local party, yet may be globally athermal due to correlations shared among different parties. Our goal is to understand how the existence of correlations distinguishes these states from true global thermal equilibrium and to compare their degrees of athermality. In particular, we ask the following questions:

1. What is the structure of a bipartite quantum state ρ_{AB} if its reduced states ρ_A and ρ_B are thermal?
2. How do correlations in ρ_{AB} evolve under global thermalisation processes, such as Gibbs-preserving operations that maintain the global thermal state?
3. How do correlations in ρ_{AB} change when only local Gibbs-preserving operations—those that preserve the local thermal states—are applied?

The project outcomes will not only deepen our understanding of fundamental physics, but also pave the path for designing more efficient quantum technologies.

Objectives

The general goal of this project is to gain a comprehensive understanding of correlations in quantum thermodynamics. To address the research questions, we set out the following objectives:

1. Identify and characterise the set of bipartite states that are locally thermal (but not globally).
2. Construct a hierarchy of these states, i.e. we say $\rho_{AB} \succ \sigma_{AB}$ if there exists a transformation $G_{AB}(\rho_{AB}) = \sigma_{AB}$ where G_{AB} is a Gibbs-preserving operation acting on the bipartite system AB.
3. Investigate how this hierarchy changes when the allowed operations are restricted to local Gibbs-preserving operations.

Research Methods

The research methodologies employed in this project are diverse. We will adopt and generalize the standard framework of quantum resource theories [7] and employ numerical techniques such as semidefinite programming [8].

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[5] F. Sapienza et al, Nature Communication 10.1: 2492 (2019).
[6] F. Binder et al. (eds), Thermodynamics in the Quantum Regime (Springer, 2018).
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Effective Hamiltonian theories for spin-phonon interactions

Electron spins can be used as physical platforms to encode qubits and qudits, but their coherence time becomes exceedingly short as temperature increases over just a few K[1]. The main culprit for decoherence in this high-temperature regime is the interaction between the spin and the lattice's phonons. Recently, the description of this complex process has become possible on a first-principles footing[2], but it requires the computation of the entire wave function of the electronic system, a complex and cumbersome physical object to work with. In this project the student will familiarize themselves with spin relaxation theory and effective Hamiltonian theories[3] in order to derive an effective spin-phonon Hamiltonian able to describe relaxation and decoherence through just a few explicit degrees of freedom. This project will require mostly analytical work, but upon successful achievement of the new formalism, there will also be the chance to perform numerical tests.

[1] Temperature- and Magnetic-Field-Dependent Longitudinal Spin Relaxation in Nitrogen-Vacancy Ensembles in Diamond. Phys. Rev. Lett. 108, 197601, 2012.

[2] The role of electronic excited states in the spin-lattice relaxation of spin-1/2 molecules Science Advances 11 (7), eadr0168, 2025.

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Learning the properties of quantum memories with equivariant graph neural networks

Atomic or molecular spins are among the most promising systems for the physical realization of quantum bits (qubits), namely the building blocks of quantum devices. However, it is imperative to design chemical systems able to support spin coherence times of several orders of magnitude longer than the current state-of-the-art in order to permit the implementation of robust quantum algorithms of practical interest. One of the main challenges in the field is to perform a rational design of new molecular units with optimal properties. The search for an optimal molecular candidate is a tough challenge due to the vast amount of possible molecular structures that can be, in principle, synthesized. Machine learning is revolutionizing science, and in this context, it might also provide powerful numerical tools for the efficient exploration of the chemical space [1]. In this project, the student will train different types of machine learning models [2-3] to learn molecular magnetic properties of critical importance for quantum applications. The student will use standard Python ML libraries (TensorFlow) to train an equivariant graph neural network to reproduce the spin Hamiltonian of a large dataset of molecular quantum memories in order to determine the most promising compound.

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[3] SchNet: A continuous-filter convolutional neural network for modeling quantum interactions, arXiv:1706.08566, 2017.

To what extent does the quantum piece-wise linearity condition apply to subspaces?

Supervisor: Prof. David O'Regan
Group: www.theoryofmaterials.com

Mentor: Andrew Burgess
Enquiries to: David.O.Regan@tcd.ie

An important and basic condition in quantum mechanics, that the total energy is piecewise linear with respect to the number of fermions in a closed system at zero temperature, is typically not obeyed by practical approximations within density-functional theory (DFT). This gives rise to all manner of problems, despite DFT being nowadays ubiquitous in practical materials and molecular simulations and every-growing. These problems include underestimated band gaps, overestimated response properties, underestimated neutral excitation energies, etc.

A commonplace remedy to this, especially for the most challenging materials, is to correct DFT with extra terms that are localised on subspaces (hence not adding much to the cost), in an effort to take out the wrong energy behaviour and put in the correct one. The strength of these corrections is sometimes measured in situ, for the system at hand. The question is, when is it safe to take conditions known to apply to a system as a whole, and apply those to subspaces?

In this project, to be performed using python/jupyter or Mathematica, we will construct a very simple model Hamiltonian, and solve it both exactly and with some standard quantum chemistry approximations. Focusing on allowing variable total and/or subspace particle count, we will seek to probe the open question of to what extent (and depending mostly on what conditions) does energy piecewise linearity hold for subspaces, which in practice interact with their surroundings? Furthermore, is there any other subspace quantity, related to the energy, which is a better target for imposing linearity? This project has the scope to improve real-world practical simulations if progress is made on this question, as will give the student experience in constructing their own simple quantum chemistry implementation from the ground up.

[1] A. C. Burgess, E. Linscott, and D. D. O'Regan, Phys. Rev. Lett. 133, 026404 (2024).
[2] A. C. Burgess and D. D. O'Regan, Phys. Rev. B 110, 205150 (2024).
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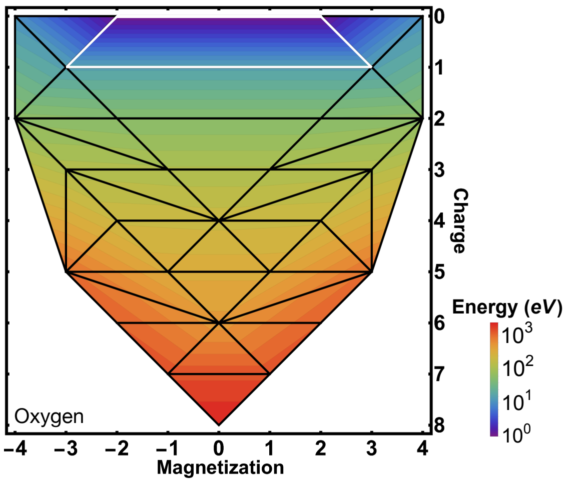

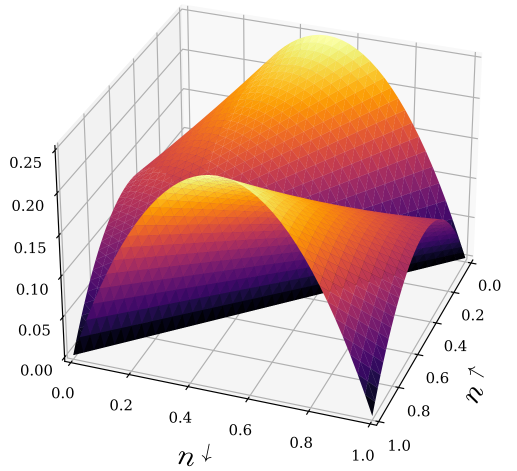

T08

Exploring novel magnetism-related systemic errors in quantum simulations.

Supervisor: Prof. David O’Regan
Group: www.theoryofmaterials.com

Mentor: Andrew Burgess
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Strongly correlated electron materials underpin diverse physical effects and technologies including high-temperature superconductivity, high-density energy storage, heterogeneous catalysis, and solid state platforms for quantum computing. While the practical computational spectroscopy of such materials is already highly advanced, the inaccessibility of their reliable total energies pushes more basic questions of their stability beyond reach. This prevents routine quantum materials discovery and design.

Continuously variable expectation values, such as for electron count, spin state, and orbital angular momentum arise in numerous commonplace theories and methods for better solving approximately for the ground state of many-particle quantum systems. This makes sense when we think, for example, of some fractional charge transfer being the first step of a chemical reaction, or the charge and spin on metal atoms in a charging battery changing smoothly as a lithium atom passes by. In finite systems, fractional particle count arises when we partition the system under study, such as to treat specific areas at a higher level of theory or to add an error correction. Increasingly, machine learning based models, based of variable particle counts, are being constructed as potential approximations to explicit quantum mechanics, targeting greater complexity.

We propose a project that will build upon our recent new exact constraints [1-2] and practical approximation schemes [3]. We will particularly focus on exploring errors in approximate density functional theory (DFT) related to spin, and how these are might be remedied in a practical way. No special prior knowledge is assumed. The project will mostly involve literature study, pen-and-paper calculations, and numerical investigations in python/jupyter or Mathematica, and hands-on DFT calculations on supercomputers.

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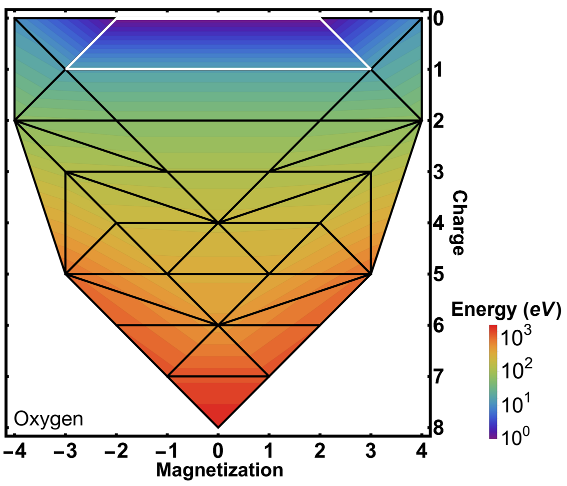
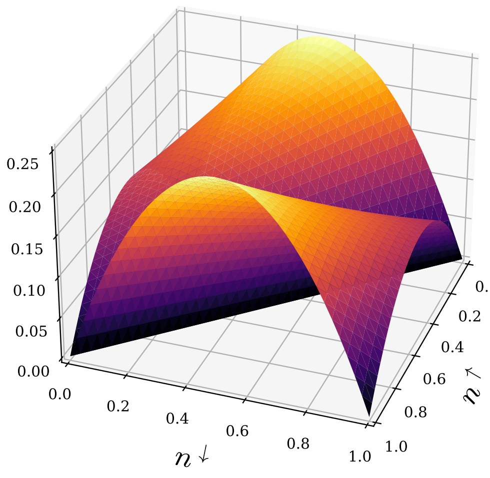
[3] A. C. Burgess and D. D. O’Regan, Phys. Rev. B 110, 205150 (2024)
[4] A. C. Burgess, E. Linscott, and D. D. O’Regan, Phys. Rev. B 107, L121115 (2023).





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

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1. Accurate modelling of diamond structure semiconductor band gaps

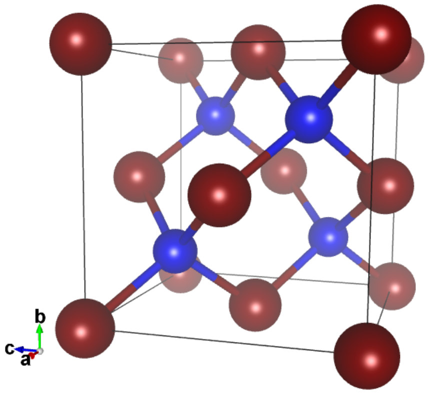

Figure 1: A unit cell of the GaAs crystal lattice, used for DFT simulations

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

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

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

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2. Linscott, E. B.; Cole, D. J.; Payne, M. C.; O'Regan, D. D., Role of Spin in the Calculation of Hubbard U and Hund's J Parameters from First Principles. *Physical Review B* **2018**, *98*, 235157.
3. Orhan, O. K.; O'Regan, D. D., First-Principles Hubbard U and Hund's J Corrected Approximate Density Functional Theory Predicts an Accurate Fundamental Gap in Rutile and Anatase TiO2. *Physical Review B* **2020**, *101*, 245137.
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Project title: Crystalline and amorphous structures in classical 2D systems: a theory perspective
Supervisor: Prof. Mauro Ferreira (ferreirm@tcd.ie)

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

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Electron motion in molecular semiconductors: quantum or classical or both?

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There are two ways electrons move in materials, which occur in different regimes of temperature. In the so-called *ballistic* regime the motion is the coherent motion of an electron across many atoms or molecules in the solid, described by the bandstructure obtained from Schrodinger's equation. In contrast, in the *hopping* regime, the electron is understood as a classical particle which is localized on an individual atom or molecule, and is kicked from place to place by fluctuations in its surroundings. These two regimes give very different results for important quantities such as the electrical conductivity. The aim of this project is to produce and study a theoretical model which unifies these two descriptions, allowing us to understand where they occur, and what might happen in intermediate regimes. The model will describe charge transfer[2] in a molecular device where charge flows around a circuit incorporating a pair of molecules (see Fig. 1). It will take the form of a simple few-level system, with states corresponding to the electrons on each molecule. You will identify the relevant equations-of-motion for the electrons, and solve them numerically using Python or Mathematica, to show how the two regimes emerge, and investigate what happens between them.

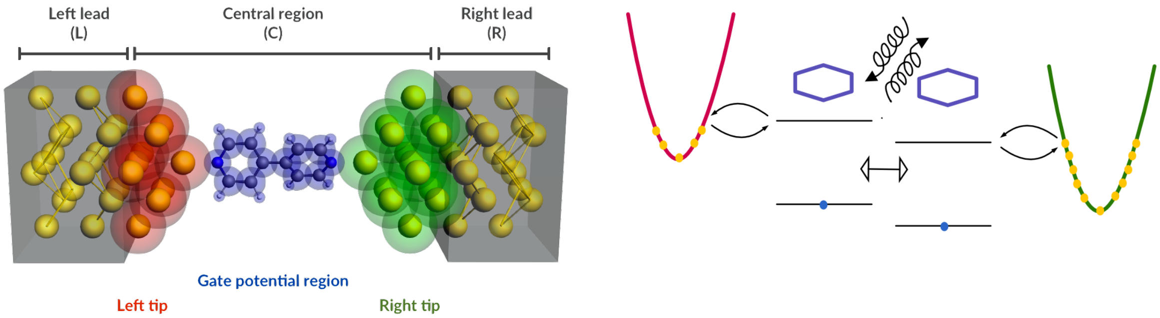

Figure 1: Left: Atomic structure of a molecular nanojunction, where charge flows through a pair of molecules between two leads. From https://www.scm.com/doc/Tutorials/ElectronicTransport/NEGFMolecularJunction.html. Right: simplified model. In the centre are the two molecules, each represented by two states, the highest-occupied molecular orbital (HOMO) and lowest-unoccupied molecular orbital (LUMO). Charges tunnel from the two leads, represented by the free electrons at the sides, and the HOMOs. They can tunnel between the two HOMO states and also release energy by coupling to molecular vibrations (wavy lines).

[1] https://www.tcd.ie/physics/research/groups/qlamg/

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Synchronization in quantum spin chains

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When self-sustained oscillators, such as clocks, are coupled together they can synchronize and tick as one[1]. This phenomenon also occurs in extended systems where oscillators are distributed throughout space and connected together, for example, between nearest neighbours[2]. These collective synchronised states are associated with a novel type of phase transition which occurs in non-equilibrium classical systems[3], and gives rise to ordered states with complex spatio-temporal dynamics. In this project you will take the first steps towards understanding how such transitions might occur for quantum systems[4]. To do this, you will develop a model of a one-dimensional chain of three-level quantum systems (spin-1), and construct the equations which describe the quantum dynamics in such a chain. By simulating small chains using Python or Mathematica, you will explore how synchronisation appears, the types of coupling that generate synchronisation, and the possible differences between the classical and quantum cases.

References

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[4] A. Roulet and C. Bruder, “Synchronizing the smallest possible system”, Phys. Rev. Lett. **121**, 053601 (2018).

Learning to Solve Physical Problems using High Performance Computing Methods

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

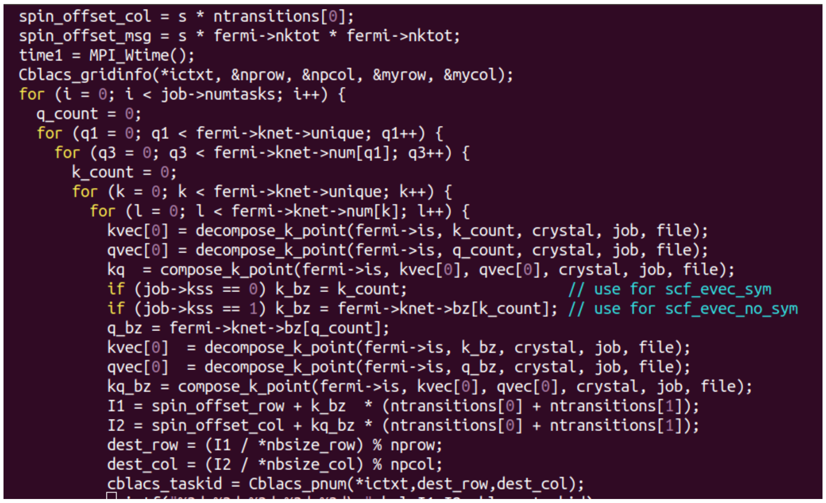
High performance computing (HPC) methods use parallel computing over large numbers of compute cores to solve large problems which are not solvable on single CPU systems. The methods include Message Passing Interface (MPI), multi-threaded computing with OpenMP and architectures such as multicore shared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

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

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

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

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



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

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

Theory and Simulation of Quantum Materials for Electroencephalography (EEG) Modelling on Flexible Substrates

Prof Ortwin Hess / Dr Illya Tarasenko

This project provides an opportunity to engage with theoretical physics, quantum materials science, and computational modelling to understand and optimize flexible, quantum-material-based technologies for biomedical and consumer electronics applications.

Motivation. Understanding the interaction of quantum materials (QMs) with flexible substrates such as skin is essential for advancing wearable electronic technologies. Quantum materials, including graphene and other two-dimensional (2D) materials, exhibit unique quantum mechanical properties that enable significant enhancements in sensitivity, signal amplification, and material flexibility. Theoretical simulations and analytical modelling play a crucial role in predicting how these materials behave at interfaces with flexible substrates, influencing the development of next-generation wearable biomedical devices. Exploring these interactions theoretically helps identify and optimize material properties and device configurations, significantly impacting fields such as medical diagnostics, neuroscience research, and consumer health monitoring.

Analytical Modelling. The analytical component of this project involves developing solutions for EEG signal propagation through multilayered, skin-like media. This begins with simplified planar geometries analogous to parallel-plate capacitor models, advancing towards incorporating quantum mechanical effects occurring at the interfaces between quantum materials and flexible substrates. Analyzing these effects is crucial for understanding their influence on signal propagation and electrode performance.

Forward Problem. Students will implement the Transmission Matrix Method (TMM) to calculate electromagnetic fields and potentials resulting from neuronal sources, initially modelled as planar dipoles. Complexity will be incrementally introduced, incorporating realistic material properties and quantum-scale interactions between electrodes and substrate layers representative of biological tissues.

Quantum Materials Interaction. The project will model quantum interactions, specifically focusing on quantum capacitance and quantum conductivity of graphene and other 2D materials on flexible substrates like skin. Students will examine how quantum material properties, such as shifts in Fermi levels and modulation of conductivity, affect EEG signal detection and amplification.

Inverse Problem. A critical aspect involves investigating methodologies to localize neuronal sources from electrode data, explicitly integrating quantum material behaviour to refine source localization accuracy. Potential ambiguities and non-uniqueness in source localization, particularly arising from multiple dipoles and quantum-enhanced detection schemes, will be thoroughly analyzed.

Resolution and Limitation Analysis. Further analysis will focus on examining how quantum material properties, electrode density, spatial arrangement, and electrode size impact spatial resolution achievable in EEG source localization. Students will determine theoretical limits and propose optimized quantum-enhanced electrode configurations to maximize spatial resolution.

Computational Implementation. Computational models will be developed using Python, MATLAB, or Julia, integrating analytical solutions with numerical simulations and quantum mechanical descriptions of electrode materials. Models will be validated against existing open-source EEG simulation tools and commercial software such as COMSOL.

Comparative Analysis. The project concludes with comprehensive comparative analyses between quantum-enhanced models, traditional analytical models, and established EEG computational tools. The goal is to assess accuracy, computational efficiency, and enhancements offered by the integration of quantum materials.

T22

School of Physics Senior Sophister Research Project 2025-2026

Electronic structure of novel bi-metal-porphyrin 2D nanonetworks

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

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

Porphyrins (Por) are organic molecules with a choice of differing divalent metal ions that can be at the center of their structure (macrocycle) giving differing band-gaps and optical spectra, examples include Fe-Por in heme and Mg-Por in chlorophyll. Porphyrin-derived nanonetworks can be formed through on-surface synthesis of halogenated porphyrin precursors resulting in networks such as in Figure 1. Adjacent porphyrins and the central metals in these can be "strongly coupled" or "weakly coupled" depending upon the covalent bridge between them. In addition, mixed metal networks can be constructed by co-deposition of e.g. differing Ni- and Co-porphyrin precursors forming a mixed (Ni/Co)-porphyrin network. What will be the electronic structure and magnetic behaviour of such a mixed system of equal Ni and Co sites? What will be the difference between a well-ordered or a disordered network?

It is envisaged that the project will use density functional theory (DFT) codes to simulate the electronic structure of these proposed mixed metal porphyrin-derived 2D nanonetworks (or 1D nanoribbons). Of particular interest will be the dependence of electronic density of states and bandstructure of the repeated central metals involved, as well as magnetic interactions. These could also be examiner where the coupling between porphyrin units differs (see Figure 1). Simulations of the manifestation of the electronic structure in observable measurements such as low-temperature scanning tunnelling microscopy (STM) are desirable. This complements our experimental on-surface synthesis work and research themes. FHI-AIMS[1] will likely be the most appropriate simulation tool.

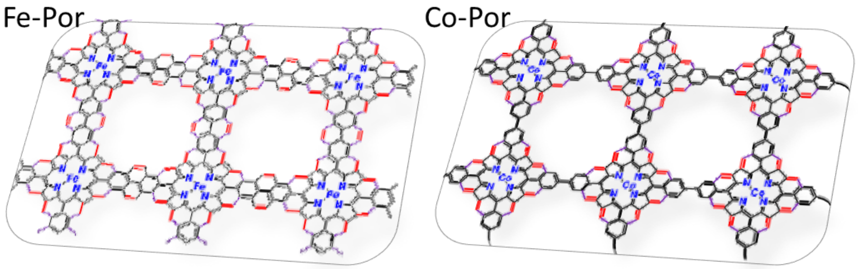


Figure 1: a "strongly" coupled uniform Fe-Por 2D nanonetwork and a "weakly" coupled uniform Co-Por 2D nanonetwork. Mixed metal networks such as Fe-Co or Ni-Co are useful to consider.

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

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

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

School of Physics Senior Sophister Research Project 2025-2026

X-ray spectroscopic simulations of one-dimensional novel 1D porphyrin nanotapes

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

The objective is to simulate the measurable x-ray spectroscopy obtainable from porphyrin-derived 1D nanotapes produced through on-surface synthesis. On-surface synthesis methods allow for the creation of entirely novel periodic nanostructures on surfaces derived from molecules rationally designed to form networks. One dimensional systems or 2D networks can be constructed from differing precursor molecules. Here precursors derived from the well-known transition metal porphyrins will introduce interesting properties of the nanostructures.

Porphyrins (Por) are organic molecules with a choice of differing divalent metal ions that can be at the center of their structure (macrocycle) giving differing band-gaps and optical spectra, examples include Fe-Por in heme and Mg-Por in chlorophyll. Porphyrin-derived 1D nanotapes can be formed through on-surface synthesis of halogenated porphyrin precursors. These can triply fuse with adjacent porphyrins at high on-surface temperatures resulting in 1D nanotapes as in Figure 1(a-b), which lead to nanotapes of differing lengths as in Figure 1(c).

X-ray spectroscopies, especially ultra high-resolution x-ray photoemission spectroscopy (XPS) and high resolution near edge x-ray absorption fine structure (NEXAFS) spectroscopy can, with complementary scanning tunnelling microscopy (STM) give specific insights into the electronic structure of these nanotapes quantifying effects of morphology and transition metals.

The project will use density functional theory (DFT) codes to simulate the x-ray spectroscopic XPS and NEXAFS measurements from these differing nanotapes that differ in symmetry of their edges and the transition metal within the porphyrin macrocycles. Calculations will use ΔSCF – or difference in self-consistent field calculations to evaluate chemical site binding energies and then establish the basis for simulating the polarisation dependent x-ray absorption spectra. Comparison will be made with existing experimental data, Figure 1(d), and predictions compared to future measurements. FHI-AIMS[1] will be the most appropriate simulation tool.

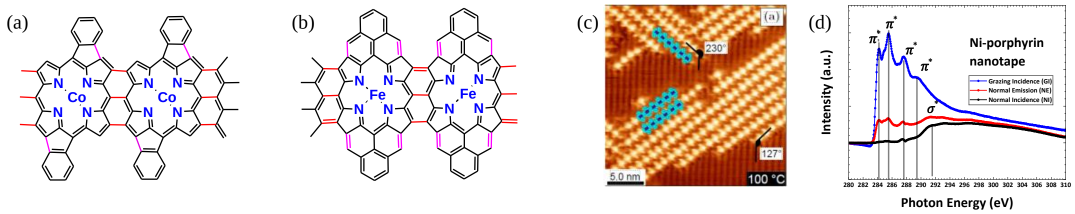

Figure 1: (a) asymmetric Co-nanotape; (b) symmetric Fe-nanotape; (c) STM of Ni-nanotape precursors; and (d) experimental C K-edge NEXAFS spectra of a Ni-nanotape measured at the MAX IV synchrotron.

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

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

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

Machine-learning the non-local non-interacting kinetic energy density

Supervised by Prof. Stefano Sanvito

Background

Density functional theory (DFT) is an in-principle exact theory to solve any quantum many-body electronic problem. The main idea is rooted in the Hohenberg-Kohn theorems [1], which establish that 1) the total energy of a many-body electronic system is a universal functional of the single-particle density, $n(\mathbf{r})$, and that 2) the functional is minimised at the ground-state density, returning the ground-state energy. For a *non-interacting system* the total energy is thus written as,

$$E[n(\mathbf{r})] = T_0[n(\mathbf{r})] + \int n(\mathbf{r})v(\mathbf{r})\mathrm{d}^3\mathbf{r}\,, \tag{1}$$

where $v(\mathbf{r})$ is an external potential (e.g. that of the atomic nuclei) and $T_0[n(\mathbf{r})]$ is the non-interacting kinetic energy. Despite this seems like a simple problem (it can be solved by solving the Schrödinger equation), in general it is actually quite difficult since an accurate expression for $T_0[n(\mathbf{r})]$ is not available. The most common approximations are rooted in a gradient expansion over the Thomas-Fermi functional, which however work well only for charge densities resembling the homogeneous electron gas (e.g. for light metals). It is now accepted that progress for non-homogeneous charge densities (e.g. for molecules) can be achieved only with non-local functionals of the form

$$T_0[n(\mathbf{r})] = \int n(\mathbf{r})K_0(\mathbf{r},\mathbf{r}')n(\mathbf{r}')d\mathbf{r}'d\mathbf{r} = \int \tau_0(\mathbf{r})d\mathbf{r}\,, \tag{2}$$

where $K_0(\mathbf{r},\mathbf{r}')$ and $\tau_0(\mathbf{r})$ are the kinetic-energy kernel and density, respectively.

Objectives

In this project we will construct machine-learning approximations to the kinetic-energy kernel for a simple one-dimensional case over a finite length. The main idea here is to use the so-called physics-informed neural networks (NN), a particular class of NNs, capable of approximating functionals [3]. The main idea is to approximate the action of a functional by expanding it over a convenient basis sets. In our case we will use the solutions of the unperturbed 1D particle in a box.

Tasks

The first task is to familiarise with the main concepts behind DFT, in particular with the problems connected to computing the kinetic energy within the DFT framework. Then, we will start constructing a numerical solver for particles in a box in 1D under a Gaussian potential using the standard particle-in-a-box functions as basis set. Then, we will implement a physics-informed neural network targeting the kinetic-energy kernel. This will be done for different number of electrons in the problem.

References

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[3] G.E. Karniadakis, I.G. Kevrekidis, L. Lu, et al. *Physics-informed machine learning*, Nature Rev. Phys. **3**, 422 (2021).

Optical Magnetic Response and the Brewster Angle

John F. Donegan and Edward Krock

1. Introduction

The p-polarized angle dependent reflection minimum resulting from the difference in the refractive index between two media occurs at the Brewster angle [1]. It has been observed in many materials and there have been many studies on it. Our group has developed a new model using multipole decomposition [2-7] and we find that the Brewster Angle equation and the Brewster condition, $\theta_{incident} + \theta_{transmitted} = 90^{\circ}$ can be derived from it. We then uncover a hidden feature of the p-polarized Brewster angle in thin films, they are only observable due to the destructive interference of the contributions of electric and magnetic multipoles. We have found that the concept of a Brewster angle can be extended to electric and magnetic quadrupoles and octupoles, showing that they too can support the zero-reflection condition. However these new Brewster angles are generally hidden due to the lack of destructive interference between other multipoles, but are required to obtain good agreement between experiment and theory. These Brewster demonstrates the possibility to support multiple p- and even s-polarized Brewster angles at different angles for the same wavelength. Our work has been verified by comparison to measurement of a SiN free-standing film measured across the visible and near-infra red wavelengths. For this project, we will carry out further computational work on the model examining materials that have small and large extinction (absorption) coefficients and also how optical gain might contribute to the observation of the Brewster angle. Some optical measurements on thin-film samples will be carried out.

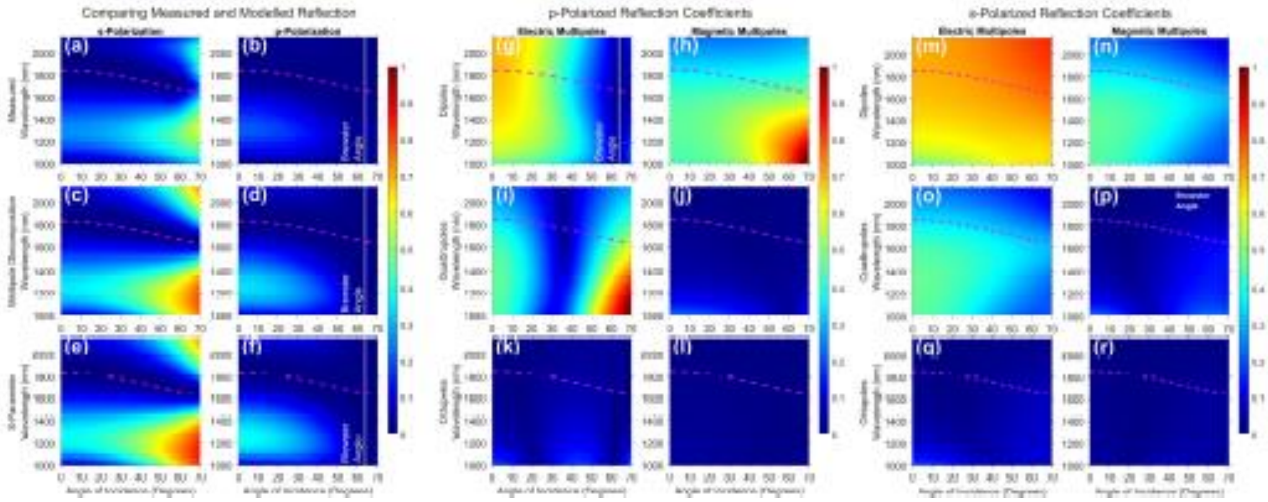

Figure: (a)-(f) Reflection from wavelengths between 1000-2145 nm and 0-70 degrees angle of incidence (g)-(l) p-Polarized Reflection coefficients over same range of wavelengths and angles (m)-(l) s-Polarized Reflection coefficients over same range of wavelengths and angles

References

[1] Brewster, David (1815). "On the laws which regulate the polarisation of light by reflexion from transparent bodies". Philosophical Transactions of the Royal Society of London. 105: 125–159. doi:10.1098/rstl.1815.0010

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T28

Project title: Sculpting the Physical properties of complex media: a multi-scale approach to material design
Supervisor: Prof. Mauro Ferreira (ferreirm@tcd.ie)

Description: Since the 1960s an ever increasing number of artists have taken inspiration from concepts developed in the sciences, frequently incorporating scientific apparatus and images in their exhibitions. The current project follows this same trend but in reverse, *ie*, with science drawing inspiration from art. Shadow sculpting is a unique art form that creates 2D shadows cast by 3D sculptures. The shadow-generating objects are made of small parts with no particular shapes and are clustered together in what looks like a pile of rubble. The figure on the right shows a few striking sculptures created by renowned artists in this field [1]. When the seemingly disordered 3D structure is probed with a light source, a specific physical response is sculpted - in this case a 2D shadow.

Fig.1- Examples of shadow sculptures - disordered objects used as a tool to design the shape of shadows

Imagine that rather than rubble we have a material whose constituents are disorderly distributed; instead of light we pass a current of a different type (*e.g.* electric, thermal or spin currents) through its structure; and in place of sculpting shadows we select whichever response we wish the material to have. In this case, similarly to finding the shape of the rubble pile that casts the right shadow, the search is for the exact material components, their respective concentrations and spatial distributions that will produce the correct physical property of our choice. This is the basic idea behind this project, *i.e.*, to use different forms of complex media to design desirable physical characteristics in a material that may or may not exist yet. This description fits into what is commonly known as *material design* but not in a conventional way because this time science will be imitating art.

The project calls for a solid background in Physics and Mathematics as well as good coding skills. Quantum Mechanics and Solid State Physics plays a major part in the project and students will have the opportunity to improve and develop their knowledge on these two subjects. A couple of useful references can be found below [2,3,4].

References:

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[3] S. Mukim, C. Lewenkopf and M. S. Ferreira, "S*patial mapping of impurities in disordered 2D materials: the conductance sudoku*", Carbon **188**, 360 (2022)

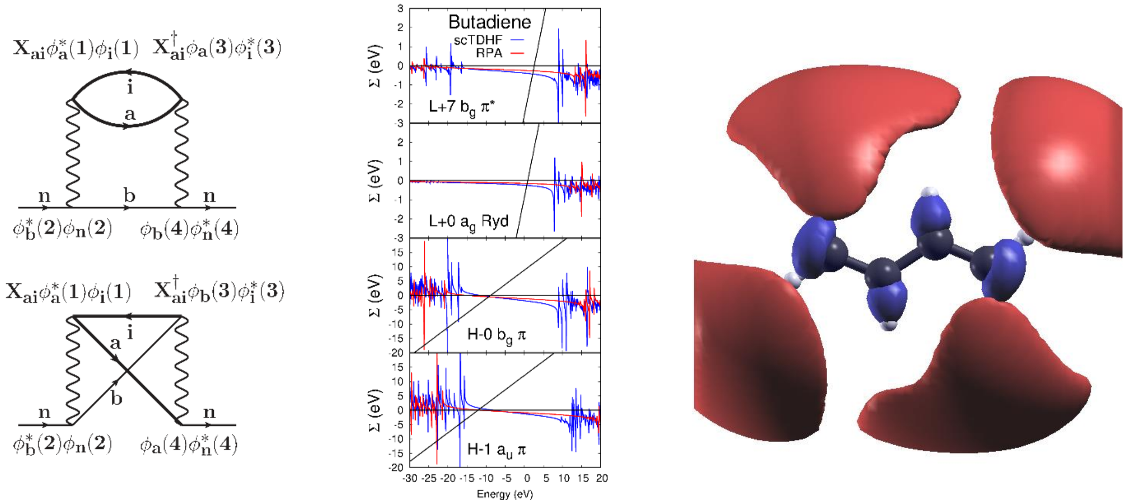
[4] F. R. Duarte, F. Matusalem, D. Grasseschi, A. R. Rocha, L. Seixas, C. J. S. de Matos, S. Mukim and **M. S. Ferreira,** *"Decoding disorder signatures of AuCl3 and vacancies in MoS2 films: from synthetic to experimental inversion"*, J. Phys.: Condens. Matter **36,** 495901 (2024)

Rydberg excited states and ionization thresholds of atoms and molecules

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

Rydberg excited states of atoms and molecules are states in which the mean distance between the excited electron and the nucleus or molecule is large, so that they are essentially an electron orbiting a positive ion. Rydberg states in which the excited electron has a specific angular momentum (S, P, D, etc), form hydrogenic series with a dissociation limit. These dissociation limits are ionization potentials of the atom or molecule.

Predicting properties such as excited state energies accurately requires a many-body approach to quantum mechanics. The GW approximation is a well- known many-body approach to calculating ionization potentials. The Bethe-Salpeter equation (BSE) is a method for calculating excited state energies. The Feynman diagrams for self-energies to be used in the project are illustrated on the left below. In this project you will calculate Rydberg excited state energies of atoms and small molecules and attempt to find the ionization threshold for various states by extrapolation to the dissociation limit. This will be compared to the ionization potential obtained directly from the GW approximation self-energies. A goal of the project will be to confirm the consistency of predicting ionization potentials by either method.



(Left) Self-energy Feynman diagrams (Centre) Energy dependence of the self-energy for HOMO and LUMO orbitals of butadiene (c) Isosurface of Rydberg LUMO orbital for butadiene.

This project will afford you the opportunity to learn about molecular quantum mechanics.

Photoabsorption Spectra of Small Na Clusters: TDHF and BSE versus CI and experiment
C. H. Patterson, [Phys. Rev. Mater. 3, 043804 (2019)]

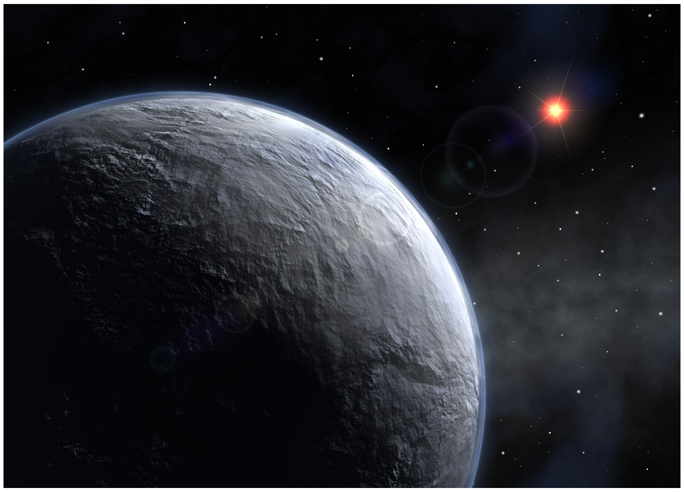
Excited states from GW/BSE and Hartree-Fock theory: effects of polarizability and transition type on accuracy of excited states,
D. T. Waide and C. H. Patterson, [Journal of Chemical Physics 161, 224108 (2024)]

Molecular Ionization Energies from GW and Hartree-Fock Theory: Polarizability, Screening, and Self-Energy Vertex Corrections,
C. H. Patterson, [Journal of Chemical Theory and Computing 20, 7479 (2024)]

Atmospheres of alien worlds: developing new models for exoplanet atmospheres

Prof. Neale Gibson
n.gibson@tcd.ie

Research Project Description:



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

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

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

References:

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

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

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

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

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

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

S. Hutzler, stefan.hutzler@tcd.ie

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

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

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