Open Dialogues across Physics & Astronomy 2023

28th – 29th March, The Open University, Milton Keynes

Book of Abstracts

Open Dialogues across Physics & Astronomy 2023

Organising committee:

Marta Podgórny - chair	The Open University
Astra Sword	The Open University
Vincent Deguin	The Open University
Timothy Leese	The Open University
Laura Blackburn	University of Sussex
Amber Shepherd	University of Sussex
Emily Ingman	University of Sussex
Daisy Shearer	University of Surrey

Special thanks to Cristobel Soares (SEPnet)

Table of context:

TIME	28th March
08:30	Breakfast - Kents Hill
09:30-10:30	Opening of the Conference Opening Keynote: Catxere Casacio
10:30-11:00	Tea Break
11:00-11:50	Discussion Panel: Open Dialogue in Physics
12:00-13:00	Lunch - Kents Hill
13:15-14:00	Student Talks: Siobhan Patrick, Natasha Bierrum, Amber Shepherd
14:00-14:50	Discussion Panel: Using Data to Answer Scientific Questions
14:50-15:20	Tea Break
15:20-15:50	Student Talks: Ashutosh Kumar Pathak, Astra Sword
15:50-16:40	Discussion Panel: Physics Outside Academia
16:40-17:30	Tea Break + Poster Session
17:30-18:30	Discussion Panel: Physics Outside Physics
19:00	Dinner - Kents Hill

TIME	29th March
08:30	Breakfast - Kents Hill
09:30-10:30	Student Talks: Agnibha Banerjee, Marta Podgórny, Kymani Armstrong-Williams, Zachary Amato
10:30-11:00	Tea Break
11:00-11:50	Discussion Panel: Having a Life Alongside Physics
12:00-13:00	Lunch - Kents Hill
13:15-14:00	Student Talks: Alexia Beale, Matthew Jones, Vincent Deguin
14:00-15:30	Closing Keynote: Pierre Ghesquierre Closing of the Conference

Invited Speakers

Dr Pamela Campbell
Earth Science
University of Glasgow

- Open Dialogue in Physics
- Physics Outside Physics

Dr Catxere Casacio
Quantum Biophysics
University of Surrey

- Opening Keynote
- Open Dialogue in Physics
- Using Data to Answer Scientific Questions
- Physics Outside Physics
- Having a Life Alongside Physics

Dr Andrew Cassidy
Molecular Physics
Aarhus University

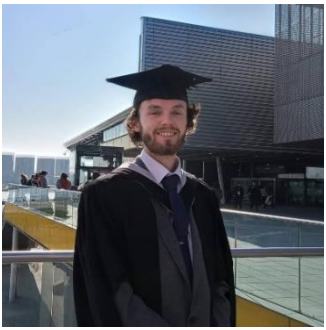
- Using Data to Answer Scientific Questions
- Having a Life Alongside Physics

Dr Anita Dawes
Molecular Astrophysics
The Open University

- Open Dialogue in Physics
- Having a Life Alongside Physics

Dr Pierre Ghesquierre
Theoretical and Computational Chemistry
Manufacture Française des Pneumatiques Michelin

- Closing Keynote
- Using Data to Answer Scientific Questions
- Physics Outside Academia
- Physics Outside Physics



Vincent Graves
Biophysics
The Open University

- Physics Outside Academia

Dr Charanjit Kaur Khosa
Particle Physics and Machine Learning
University of Bristol

- Using Data to Answer Scientific Questions
- Physics Outside Physics

Dr Annika Lohstroh
Nuclear Solid-state Physics
VacuTec Meßtechnik GmbH

- Open Dialogue in Physics
- Physics Outside Academia

Participants

Oral presentations:

Zachary Amato
Kymani Armstrong-Williams
Natasha Bierrum
Agnibha Banerjee
Alexia Beale
Vincent Deguin
Matthew Jones
Ashutosh Kumar Pathak
Siobhan Patrick
Marta Podgórny
Amber Shepherd
Astra Sword

Posters:

Kymani Armstrong-Williams
Alexia Beale
Vincent Deguin
Matthew Jones
Annie R Lennox
Marta Podgórny
Yojana Rai
Amber Shepherd
Astra Sword

Structure-properties relationships in polymer nanocomposites: applications to tyre thread materials

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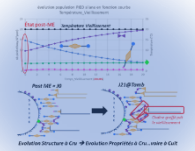
Innovation in the field of tyres is a major concern in order to offer ever more efficient materials while limiting fuel consumption and CO_2 emissions. In this context, the control and understanding of the phenomena that govern the structure of elastomer-type materials reinforced by nanometric fillers (silica or carbon black) are crucial issues for optimizing the macroscopic properties of the corresponding composites.

To achieve these objectives at Michelin, we have internally developed a chain of simulation software at the mesoscopic scale to predict the elementary mechanical properties (rheology and dynamic properties) of nanocomposites from the structural variables identified in experimental work. A first brick uses a population-balanced model [1] to describe the evolution of the polymer's macrostructure, dispersion, and distribution of reinforcing fillers from the micrometer to the nano-metric stage, and the reactivity of the polymer-filler coupling agent. A second brick is a coarse-grained molecular dynamics code [2] that allows to predict the relaxation modulus of the material from the dynamics of the entanglements of the polymer within the nanocomposite and to calculate the effective interaction mediated by the matrix on the nanoparticles, therefore, to predict the 3D organization of nano-objects within the material. A third brick finally aims to simulate a realistic structure of the network of reinforcing fillers [3], and to use the interaction potential previously described to simulate the physical, mechanical and dynamic properties of the system.

We will present how we can describe the mechanical and rheological properties of these systems from the formulation/process couple, through an understanding of the system structure and multi-scale modeling.

COFRA



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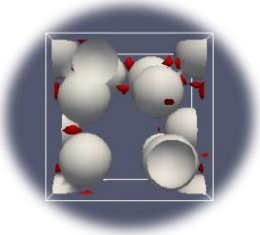
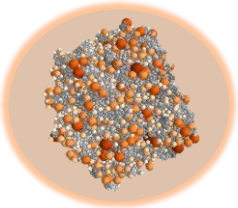


MESOSCOPE



Mots-Clefs: *Reinforced Elastomers, Population-Balanced Model, Coarse-Grained Molecular Dynamics*

References:

[1] D. Ramkrishna, 'Population balance modeling: Current status and future prospects', Annual review of Chemical and Biomolecular Engineering, 5, p123-146, 2014

[2] D. Del Biondo, E. M. Masnada, S. Merabia, M. Couty, and J-L. Barrat (2013) Numerical study of a slip-link model for polymer melts and nanocomposites J Chem Phys. 138, 194902.

[3] Yang Wang, Gaëtan Maurel, Marc Couty, François Detcheverry, and Samy Merabia, Implicit Medium Model for Fractal Aggregate Polymer Nanocomposites: Linear Viscoelastic Properties, Macromolecules 2019 52 (5), 2021-2032

Exploiting Neutrons to Unveil Star-Formation: Exploring Dynamical Amorphous Ice Systems

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Interstellar ice, dominated by Amorphous Solid Water (ASW), is the largest molecular reservoir in the Universe. In planet-forming disks, the dominant formation mechanism of ASW is vapour deposition of H2O from the gas-phase onto dust particles. At low temperatures (≤ 80 K), the ASW is usually very porous, allowing for a large number of molecules to be stored within these pores. However, it seems that meta-stable interstellar ASW loses porosity as a function of time or temperature as star-formation progresses. This porosity change is astrochemically vital as it alters the total ASW surface area, affecting the chemistry that can occur on/within the ice and how the icy grains might "stick" to form the early seeds of planets The overarching aim of our research is thus to understand the thermally induced changes in the physical properties and structure of these ices.

Over the past decade, our group has employed NIMROD and SANS2D at the ISIS Neutron and Muon Source to study ASW growth and thermal evolution with neutrons. From our current data, it is clear that our vapour-deposited ASW exhibits both granularity and porosity- both of which evolve as a function of temperature. To get an atomistic understanding, we have also developed molecular dynamics code to simulate the annealing of vapour-deposited water-ice using GROMACS.

The Double Copy: A Duality for Particles and Gravity

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An open problem in theoretical physics is to combine all four of the fundamental forces of nature into one single theory. Problematically, gravity has proven difficult to reconcile with the other forces. Recently, relationships between scattering amplitudes (the quantity related to the probability for an interaction to occur between two or more particles) in non-abelian gauge theories (such as the theory of quarks and gluons) and theories of quantum gravity have led to the discovery of a relation known as the double copy. The double copy relates scattering amplitudes in quantum gravity as the square for those in non-abelian gauge theories. This property has been extended to relate solutions in classical electromagnetism with those in general relativity, via a theory known as the classical double copy.

Keywords: *Gravity, Particle Physics, Quantum Field Theory*

Fast-Spinning Planets and their Inflated Atmospheres

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Transmission spectroscopy is a highly effective method for studying exoplanet atmospheres [1]. Understanding exoplanet atmospheres using this method consists of generating numerous models and comparing them to observations. One common assumption in these models is that the planet is a non-rotating, isolated sphere. However, this assumption overlooks the impact of a planet's rotation, which raises the scale height of the atmosphere due to centrifugal force. In this work, we use the retrieval code NEMESIS [2] to quantify the effect of this assumption on the atmospheric properties retrieved using this technique. Our findings show that conventional atmospheric models used for retrievals may produce different results for close-in, low-gravity planets when this assumption is not taken into consideration. These differences can affect our understanding of the atmospheres of close-in hot Jupiters being observed by JWST.

References:

[1] Charbonneau, D., Brown, T.M., Noyes, R.W. and Gilliland, R.L. (2002). Detection of an Extrasolar Planet Atmosphere. The Astrophysical Journal, 568(1), pp.377–384. doi:10.1086/338770.

[2] Irwin, P.G.J., Teanby, N.A., de Kok, R., Fletcher, L.N., Howett, C.J.A., Tsang, C.C.C., Wilson, C.F., Calcutt, S.B., Nixon, C.A. and Parrish, P.D. (2008). The NEMESIS planetary atmosphere radiative transfer and retrieval tool. Journal of Quantitative Spectroscopy and Radiative Transfer, 109(6), pp.1136–1150. doi:10.1016/j.jqsrt.2007.11.006.

Colloidal Gelation Inside Porous Structures Imaged Using X-ray Computed Tomography

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The coating of porous substrates is useful for applications in wastewater treatment, catalysis, and filtration. High porosities provide a large surface area for interfacial reactions. In the coagulant gelation method of coating, a charge-stabilised colloidal dispersion is spread on a substrate decorated with salts that dissolve and destabilise the colloid to create a gel layer. We propose to coat the interiors of pores using the coagulant gelation process while filling them via capillary action. The challenge is to coat the interior walls uniformly without fully plugging the pore with a colloidal gel. As a model porous system, bespoke substrates with well-defined straight channels (1mm radius) are fabricated using 3D printing of poly(lactic acid). We employ the technique of X-ray Computed Tomography to image the coating of channels within opaque substrates.

Our initial results show that the coating thickness within the model porous structure is dependent on the concentration of coagulant for both a monovalent and a divalent coagulant. We found that the thickness of the coating at the base of the channel is consistent with the model developed by Williams *et al.* [1], which predicts that the gel thickness is non-linearly dependent on the coagulant concentration. We have demonstrated that the channels may be coated using the coagulant gelation process without plugging. We also discovered that adding nanoclay to increase the porosity of the coating beneficially provides X-ray image contrast between the substrate and the coating.

This work will open up possibilities for future design of substrates for biocatalytic coatings, which may be applied to processes including wastewater treatment and bioprocessing. Future research will explore more complex 3D structures and investigate the functionality of the coatings.

References:

[1] Williams, I., Naderizadeh, S., Sear, RP. and Keddie J.L. (2022). Quantitative imaging and modelling of colloidal gelation in the coagulant dipping process. The Journal of Chemical Physics, 156(21), pp.4905. doi:10.1063/5.0097297

Radio-frequency dressing modification of Bose-Einstein condensates

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Bose-Einstein condensate (BEC) is a state of ultracold matter where many individual atoms form a macroscopic quantum object, whose characteristics of constant phase across the cloud and calculable density make it an ideal tool for studying quantum phenomena. The applications range from answering fundamental questions on the quantum mechanical world, to quantum sensors for gravity and current paths. In our experiment BECs are made on an atom chip from the magnetic fields that are produced from the micro-wires, and a radio-frequency is applied to modify the magnetic potential, called the dressing radio-frequency. The atom chip gives a high amount of tuneability and control over the trapping potential. Specific parameters of the trapping potential give control over the phase, interaction strength of the atoms, and dimensionality of the BEC. The addition of a radio-frequency dressing field creates an avoided crossing in the energy levels and allows for coherent splitting into multiple BECs. Control over the radio-frequency switching on and off, and length of time dressing is important for adiabatic modification and so that it has no adverse effects on the properties of the BECs. The effect of the radio-frequency field is studied by investigating the frequencies of the magnetic traps, the interference of the BECs due to the change in phase and FFT results of optical density images. Multiple radio-frequency potential has not been achieved on an atom chip before, and we discuss how the results will inform creating three or more BECs at once chip and how the relative phases can be studied.

Keywords: *Bose-Einstein condensates, lasers, ultrahigh vacuum, radio-frequency*

Presentation of my online research notebook

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Motivation
Taking reliable scientific notes has always been a big struggle for me, and yet it is a very important aspect of the scientific method. After years of investigations and experimentation, I can proudly say that I have found a solution that works for me in that regards, and many many more ...
Methodology
Moving away from the classical pain and notebooks, I have started taking notes using markdown. With the help of Jupyter Book, a collection of markdown files can be converted to HTML. Resulting from this process is a perfectly working website with very little effort (that can be hosted for free on Github). This is a game changer for making science more open, transparent, and reproducible as well as promoting an Open Dialogue between scientific disciplines.
Research Findings
The results I obtained are available at the following adress:
- https://deugz.github.io/nb-master/_build/html/intro.html
Conclusions and Impact
It is now possible to directly convert scientific notes into a perfectly working website (easily). This can have a massive impact in many different research areas including overcoming the academic publishing business, promoting an open dialogue between researchers of various disciplines, and allowing for a more creative way to produce teaching material.
Link to other fields: *Every researcher, from all disciplines could benefit from adopting this novel methodology.*

Modelling the time evolution of the scattering intensity during polymeric spinodal decomposition using dynamic mode decomposition

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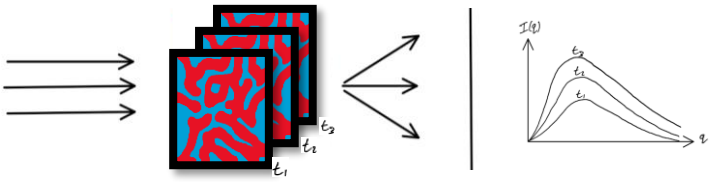
Scattering experiments are a powerful way to probe the evolution of the microstructure in heterogeneous materials, for example, immiscible polymer blends. In spinodal decomposition – the process of spontaneous demixing following a temperature or pressure change – information about the microstructure can be deduced from measurements of the scattering intensity [1; 2]. While the time evolution of the scattering intensity can be measured relatively easily, modelling it has proved to be much more difficult [3] Embracing this duality, we model the time evolution of the scattering intensity in simulated polymer blends using dynamic mode decomposition [4], a data-driven modelling algorithm. We assess the accuracy and range of the predictions and investigate the parameter choices required to build good models. Our findings suggest that dynamic mode decomposition could be used practically and effectively to make future predictions of the scattering intensity in an experimental setting.



Keywords: *polymer blends, phase separation, data-driven modelling*

References:

[1] Higgins, J.S. & Benoit, H.C. (1994), Polymers and Neutron Scattering, Oxford University Press
[2] Jones, M. & Clarke, N. (2021), Machine Learning Real Space Microstructure Characteristics from Scattering Data, Soft Matter, 17(42): 9689-9696
[3] Akcasu, A.Z. et al. (1992), Theoretical and Experimental Study of Dissolution of Inhomogeneities Formed During Spinodal Decomposition in Polymer Mixtures, The Journal of Chemical Physics, 97(8):5782-5793
[4] Brunton, S.L. & Kutz, J.N. (2016), Dynamic Mode Decomposition, SIAM

Data Entry Hackathon(s) on Space Science Nomenclature

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Motivation
Following on from my talk on a similar topic at last year's OPaPA, myself and individuals from the University of Southampton's Women in Physics Network organised the first in what will be a series of hackathons exploring the eponyms of named features across the solar system. This work was started after I had noticed a significant gender imbalance in named surface features on Mercury. The hackathon aims to show that this lack of diversity is not simply an issue of gender, and is not unique to Mercury but rather diversity is lacking across the solar system.

Methodology
Conventions, as set and maintained by the International Astronomical Union, dictate the names surface features may adopt. We separated these conventions into three categories: those in which the names of people (real or mythological) were used, the names of places were used (real on Earth or non-real), or the names of objects were used. We analysed the eponyms of named features to explore a range of diversities; including, but not limited to, the distribution of gender, sexuality, nationalities and ethnicities, and geographical distribution. We also noted the years in which features were named, hoping to see a trend towards better diversity in more recent years.

Research Findings
At the moment, we are around a third of the way through the IAU's extensive database of named features. We have so far confirmed a bias towards the names of cis white European men, and discovered some intriguing inconsistences with the conventions themselves.

Conclusions and Impact
Ultimately, I want to present this work to encourage more people to be a part of the effort. Exploring the database of named features is time consuming and arduous for one person, and the more people involved the better. The aim in publishing these results is to lobby to the IAU to have conventions changed such that in future it is easier achieve better diversity within planetary science nomenclature.

Link to other fields: *I firmly believe that all research has an EDIA implication. The whole field of physics is no stranger to the history of the underrepresentation of women. It was a gender imbalance I initially recognised in this work, but as I said, this is not limited to an issue on gender and there are many forms of diversity that are lacking.*

Free-Text Sub-questions of The Force Concept Inventory: An Effort to Make it a More Effective Tool

Ashutosh Kumar Pathak[1], Dr Jonathan Nylk[1], Prof Sally Jordan[1]
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Students often come in the classroom with preconceived ideas based on their kinesthetic memories and what they have experienced in their daily lives. Force and motion are among the concepts that are vastly dissimilar from intuitive thinking. When viewed from a factual perspective, the meaning of these concepts alters. “Students’ preconceived ideas have a significant impact on physics education but cannot be determined without thorough research”. Consequently, several diagnostic tools have been developed to assess students’ understanding.

The Force Concept Inventory (FCI) [1] is one of the tools used to gauge students' basic understanding of Newtonian mechanics. It consists of 29 multiple choice questions which probe six Newtonian concepts. Each question has five options; one of the options is true and four are closely related distractors. The purpose of the FCI is to probe alternate conceptions/ misconception in Newtonian mechanics. It is commonly used for assessment and research purposes.

The structure of each FCI item is such that it requires a forced choice between Newtonian concepts and common-sense alternatives. Incorrect answers/distractors provide more information about students’ alternative beliefs. In order to investigate students’ understating of Newtonian mechanics, each item needs to be given equal attention.

The free-text version of the FCI will be explored in the research talk. Free-text questions, as opposed to multiple-choice questions, can significantly reduce the probability of guessing and aid in understanding students' alternative conceptions. Questions have been reframed so as to require an answer in the form of an automatically marked phrase or sentence (using the Moodle Pattern Match question type), continuing the work of Mark Parker (2019) [2].

Reframing the FCI in a free-text format presents several challenges in the interpretation of student responses and identification of misconceptions. Parker’s work will be broadened to the use of free-text sub-questions in the FCI, giving improved diagnostic capability for gauging students' understanding of Newtonian mechanics

Keywords: *Force Concept Inventory, Misconceptions, Physics Education Research, Newtonian Mechanics*

References:

[1] Hestenes, D., Wells, M., & Swackhamer, G. (1992). Force Concept Inventory. The Physics Teacher, 30(3), 141-158. DOI: 10.1119/1.2343497

[2] Parker, M. (2020) "Establishing Physics Concept Inventories Using Free-Response Questions" (PhD Thesis) https://oro.open.ac.uk/73254/

COLD ATOMS FOR QUANTUM COMPUTING

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The aim of this work is to demonstrate high levels of control over neutral atoms in optical traps with a view to using them as qubits in a quantum computer. Quantum computers have the potential to have a large impact on society. Quantum properties like entanglement and superposition mean quantum computers would be able to solve some problems which classical computers aren't able to, such as the simulation of complex molecules in the development of medicines.

In our lab, we cool atoms to around 90 µK and trap them in a micron sized trap. I am currently working on characterising this trap, but in the future, we hope to demonstrate manipulation of the state of the atom, particularly excitation to the Rydberg state (very high energy levels). Rydberg states and a phenomenon known as Rydberg blockade provide the mechanism we hope to use to perform conditional logic gates, such as the CNOT gate, on the atoms in the trap. The CNOT gate is one of the fundamental building blocks for quantum computation, hence its demonstration in the cold atom platform is an important proof of concept.

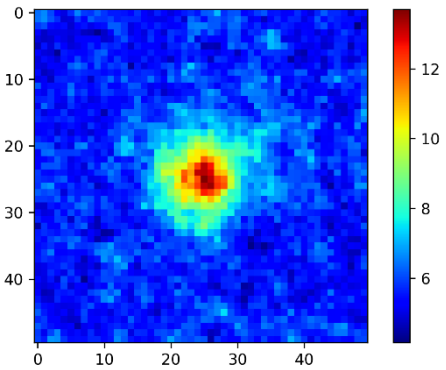

Figure 1. Image of approximately 22 atoms taken 10 µs after they are released from the trap. Image is composed of 750 frames added together.

Keywords: *Quantum technologies, atoms, dipole trap*

References: [1] Mansell, C. W. and Bergamini, S. (2014), 'A cold-atoms based processor for deterministic quantum computation with one qubit in intractably large Hilbert spaces', *New J. Phys.* 16, 053045

Investigation of the influence of the ice formation temperature on spectroscopic properties of methanol ice

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Methanol had been in the interest of interstellar studies due to its role in ice evolution. As a simple organic compound, CH3OH can be a component in many reactions leading to compounds such as methane, formaldehyde, ethylene glycol, or dimethyl ether [1]. However, not only is methanol's reactivity worth further research, but also its structure. With the first phase transition at the temperature of 103 K [2], methanol ice can occur both in the amorphous, and crystalline form [3].
As there is still a lack of detailed, systematic studies on methanol ice's properties, this research is focused on its crystalline structure as a function of temperature. In this study, CH3OH ice layers were grown at temperatures from 98 K to 125 K to analyse how high-temperature deposition influences the crystalline structure and the process of crystallisation.
For analysis of the methanol ice structure, three vibrational modes were chosen – OH stretch, CO stretch, and CH3 in-plane rocking as indicators of phase transition. It was observed that depending on ice formation temperature, differences in mid-infrared spectra were visible which shows applicational potential for studies of thermal history and more detailed astronomy observations.

Keywords: *ISM, methanol, ice crystallisation*

References:
[1] Schmidt, F., Swiderek, P., & Bredehöft, J. H. (2021). Electron-Induced Processing of Methanol Ice. ACS Earth and Space Chemistry, 5(2), 391–408. https://doi.org/10.1021/ACSEARTHSPACECHEM.0C00250
[2] Dounce, S. M., Mundy, J., & Dai, H. L. (2007). Crystallization at the glass transition in supercooled thin films of methanol. The Journal of Chemical Physics, 126(19). https://doi.org/10.1063/1.2741506
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Spin Physics in the Action of Isoniazid Drug

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Motivation

Isoniazid (INH) is the oldest synthetic drug and has been used as the frontline treatment of tuberculosis (TB) caused by Mycobacterium Tuberculosis (Mtb). Due to the rise of multi-drug resistance (MDR), TB still remains a threat to public health. INH is oxidised in the cell walls of Mtb bacteria by the catalase-peroxidase katG gene to generate a strong inhibitor of InhA (an enzyme essential for mycolic acid biosynthesis). Some preliminary work carried out by Prof. Graham Timmins in the University of New Mexico has suggested that there might be some magnetic-isotopic effect on these InhA inhibitors.

We will be Investigating these spin effects in INH and if evolution has made use of quantum effects.

Methodology

Activate Isoniazid in-vitro by Mn(III) and in-vivo by katG and investigate magnetic field effects. [13C] labelled INH will be used for oxidation assays by either Mn(III) or katG. The oxidised INH will be subjected to magnetic field and samples will be analysed with HPLC and Mass Spectrometry.

Link to other fields: *We will be able to establish that biological systems do utilise quantum mechanics and use this knowledge in improving drugs development and many other medical applications.*

Building a molecular nitrogen clock for fundamental physics

Amber Shepherd[1], Laura Blackburn[1], Matthias Keller[1]
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Motivation
To search for time-variations in the proton-to-electron mass ratio in order to test the limitations of the Standard Model and search for new physics.
Methodology
Quantum clocks use highly precise transitions in atoms and molecules to accurately measure time. The frequencies of some transitions used in quantum clocks depend on fundamental constants, such as the fine structure constant and the proton-to-electron mass ratio. Hence, measured changes in these frequencies could indicate variations in those fundamental constants. This experiment will use a Raman transition in a molecular nitrogen clock to probe these possible time variations. Currently, a network of clocks with different dependencies on fundamental constants are being set up to form a network which can be used to cross-reference data.
Research Findings
So far, some Ti:Sapph lasers have been set up to ionise nitrogen. Ti:Sapph lasers can achieve high energies and narrow linewidths, allowing high efficiency ionisation.
Conclusions and Impact
Some extensions to the Standard Model predict different variations in fundamental constants; some predict a slow drift, and others a fast oscillation, for example. By characterising any changes in fundamental constants, this will indicate where the limitations of the Standard Model lie, as well as which alternative theories are best to pursue.

Keywords: *Ion traps, photonics, quantum technologies*

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