Plenary talk

*Be Revolutionary: Change the world*

Prof. Sir Colin Humphreys

13:30 - 14:30

Abstract

According to Stephen Hawking, the human race faces mass extinction within the next 100 years. Is he likely to be correct? How would Sir Winston have probably responded? Will robots and Artificial Intelligence be a blessing or a curse? How should we respond? Can we have the vision to change the world?

Biography

Colin Humphreys is Professor of Materials Science and Director of Research in the Department of Materials Science and Metallurgy, University of Cambridge, and a Fellow of Selwyn College, Cambridge. He is a Fellow of the Royal Society and a Fellow of the Royal Academy of Engineering. He was knighted in 2010 for “services to science”. He founded and directs the Cambridge Centre for Gallium Nitride (GaN). He founded two spin-off companies to exploit the research of his group on low-cost LEDs for home and office lighting. The companies were acquired in February 2012 by Plessey, which is now manufacturing LEDs based on this technology at their factory in Plymouth, UK. He founded and directs the Cambridge/Rolls-Royce Centre for Advanced Materials for Aerospace. He recently founded a new company, Paragraf, to exploit the research of his group on graphene. In his limited spare time he writes on science and religion and is the author of *The Miracles of Exodus* (Harper Collins, 2003), which has been translated into German and Portuguese and has an Audio edition, and *The Mystery of the Last Supper: Reconstructing the Final Days of Jesus* (Cambridge University Press, 2011), which has been translated into Russian, German, Portuguese, Japanese and Greek, and has a South Asian edition.
**Are black holes heating up dwarf galaxies?**

Sophie Koudmani

Heat plays a major role in how galaxies grow. It is needed to prevent the galactic gas from immediately clumping and forming an excessive number of stars. For large galaxies, the most powerful heating emanates from matter falling towards the black holes found in their centre. Until recently, astronomers thought that small galaxies (so-called dwarf galaxies) did not have massive black holes at their centre. This meant that these galaxies would only have the significantly less energetic heat from supernovae (big explosions at the end of a star's lifecycle) to slow down star formation. New observations have shown that this canonical picture of heating mechanisms is incomplete: at least 1% of dwarf galaxies do have central black holes. However, these black holes are much lighter than their supermassive counterparts in large galaxies. Therefore, it is uncertain whether they would be able to prevent gas from forming stars. To resolve this question, I have set up high-resolution computer simulations of dwarf galaxies. Here I will present the results from the simulations and demonstrate for which types of dwarf galaxies the black hole dominates the heating. I have found that the effect of black hole heating in dwarf galaxies is hugely important and a missing piece in our understanding of the Universe.

**Understanding Expectation Propagation through toy examples**

Siddharth Swaroop

In the field of machine learning, approximate inference is becoming increasingly important due to increasingly larger and more complex models and data. Out of the many approximate Bayesian inference methods, expectation propagation (EP) is an algorithm often found to work well in practice (for example, it is used in the Xbox ranking system). However, it can sometimes fail, and its properties are poorly understood. By applying EP to some well-chosen toy cases, we can build a picture of why and when EP would work well on larger models.

**Solid State Ion Conductors for Next Generation Batteries**

Jack Hodkinson

Currently state-of-the-art battery technology relies on organic electrolytes which are flammable and have a limited operating voltage. Solid state electrolytes are a safer alternative and could allow for the production of batteries with a longer lifetime, however, only a handful of solid ion conductors are known to exist. This research focuses on the synthesis and characterisation of novel solid state electrolytes and explores the relationship between their atomic structure and electrochemical performance.
Contactless Smartcard Distance-Bounding Protocol Security Analysis

Dominic Celiano

Contactless smartcards are commonplace for applications such as access control and payment systems. However, commonly used cards, such as the Mifare Classic, have already been shown to be insecure. To improve security and prevent relay attacks, distance-bounding protocols have been implemented in many contactless smartcards, including the Mifare Plus EV1. In this project, the security of the Mifare Plus EV1’s distance-bounding protocol was analysed by implementing a Mifare Plus reader and using the reader to overclock the Mifare Plus EV1. The reader was implemented on the Proxmark 3 hardware development platform.

How do companies incorporate sustainability considerations into their decision-making?

Catherine Tilley

In 2015, through the Paris agreement and the Sustainable Development Goals, we described the world we want to see. Business plays an important role in transitioning to this new world, and there are pressures on large incumbent businesses to become more environmentally and socially sustainable. But sustainability is enacted. It is the outcome of hundreds of decisions taken by people every day at all levels from the strategic to the operational. Many of these decisions are taken routinely, without much thought, in ways that are embedded in the structures of the organisation. Introducing sustainability considerations often introduces tensions and makes decision-making more complex, for example requiring new data, ways of looking at problems or organisational systems for decision-making. My research explores the way in which people in organisations are making decisions about social and environmental sustainability, and how organisations can change to make it easier for people to ‘do the right thing’.

Tracking wakefulness in the fly brain

Sridhar Jagannathan

It has been more than 175 years since the first use of general anaesthetics in surgery, however the mechanisms through which it works it not yet known. In fruit fly (Drosophila melanogaster) it has been shown that volatile anaesthetics activate the sleep pathways before producing analgesic (pain free) functions. Hence it is important to understand the brain mechanisms behind falling asleep in fruit flies. Till recently, sleep in flies has been detected by absence of movement (video recordings) for more than 5 minutes. Recently, we developed mathematical methods based on brain data recorded from flies and detected fly sleep independent of movement. We were able to detect fly sleep 2 minutes prior to initiation of no movement and further able to predict the duration of sleep in this period. These findings form an important first step in understanding the mechanisms behind falling asleep.
Network Latency in Data Centres: Measurement, Impact and Mitigation

Diana A. Popescu

In this talk, I will explain how to measure network latency in data centres and show why network latency matters and how it impacts application performance, and how we can improve cluster scheduling to take into account network latency application requirements.

Discovering Novel Materials for Energy Storage Using Computational Techniques

Angela F. Harper

The growing need for sustainable and efficient energy storage devices demands research into rechargeable batteries, specifically lithium-ion batteries, which currently dominate the battery research field due to their high energy density. However, this technology at the present state contains two main limitations: first, the dwindling abundance of Li which has led to steep increases in cost, and second by the efficiency of the electrode materials used. Sodium-ion batteries have thus received increased attention in recent years, given the relatively high abundance of Na. Given that Na+ ions have a larger radius than Li+, attention must be given to the choice of suitable anode materials, which allow for adequate sodiation. To address both issues, an automated computational approach is employed which predicts novel anode materials with higher capacities from first principles calculations.

The ab initio Random Structure Searching code (AIRSS) is used to search for the initial anode structures, and a ternary hull is constructed between these compounds and either Li or Na. The structures which lie close to the hull, and thus are most energetically favorable are then further studied as a means of understanding the chemical transformations undergone during lithiation or sodiation. AIRSS can then be used to predict the structures formed both at the interface between these anodes and an electrolyte, and within the grain boundaries of the bulk materials. From this high-throughput method we can understand the chemical pathways of ion conduction in novel battery materials and calculate energetic barriers at the anode-electrolyte interface.

The Everett and Copenhagen interpretations of Quantum Physics: a comparison

Sivapalan Chelvaniththilan

In this presentation, I will review the two main interpretations of Quantum Physics and the research work done by Frauchiger et al (2016), Deutsch (1984), Wigner (1952) and Carroll et al (2015) on whether it is possible in principle to determine which one of them is the correct interpretation. I will also review works that explore the implications of this to the field of thermodynamics.
Materials simulation from the ground up

Max Veit

Since the invention of quantum mechanics in the 1920s, physicists have dreamed of using these equations to describe how our everyday world works. They have been incredibly successful in describing the sub-microscopic world — molecules, atoms, and subatomic particles. But Dirac foresaw the problem as early as 1929: "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble" [1]. In fact, the equations of quantum mechanics are too difficult to solve exactly on anything more complicated than a hydrogen atom! Luckily, the invention of the computer along with decades of diligent work has given us algorithms for approximate methods of solving these equations, which has allowed us to progress to crystals (because of their periodic structure) and molecules as large as DNA. Liquids, on the other hand, are more difficult because of their lack of order. Other, empirical approximations are employed for liquid simulation, but these must be fitted to measurements we've already done! Only recently have scientists been using machine learning techniques to get the best of both these worlds: The rigorous accuracy of quantum mechanics together with the efficiency of empirical potentials. In this talk I'll present my work on using this approach to make accurate, faithful simulations of liquid methane, the simplest alkane. I'll show how these simulations help us achieve that long-sought goal of predicting its macroscopic properties from real fundamental physics. We hope this approach will lay the foundation for a new generation of true first-principles predictions for a wide range of liquids of scientific and industrial importance.


Learning distributed word representations

Richard Ngo

An important issue in natural language processing is the question of how to represent the meanings of words. One successful approach has been to learn embeddings in a high-dimensional vector space. The principle underlying this approach is the distributional hypothesis: that a word's meaning can be characterised by the contexts in which it appears. It has been shown that embeddings based on the distributional hypothesis do reflect actual semantic similarities.

While word embeddings are usually calculated using distributional data for original words, some modifications - for example by removing the suffixes of words before using them as inputs to a neural network - can improve the ability of neural networks to recognise synonyms. However, there has been little work on how varying the embedding type affects sentence-level tasks such as paraphrase detection. My research involves training neural networks to detect sentences with similar meanings (paraphrases), and evaluating whether adding grammatical or morphological information about the words involved can improve performance. This is a step towards making word representations more easily interpretable by humans.
Exploring Large-scale Conformational Changes in Proteins

Jerelle A. Joseph

Large-scale structural transitions in proteins often involve multiple degrees of freedom. Therefore, it is usually difficult to simulate these transitions at biologically relevant time scales using conventional computer simulation techniques. The potential energy landscape (PEL) framework represents an attractive alternative for characterising the structural features, thermodynamics and kinetics of such transitions. This approach utilises geometry optimisation, which is inherently time-independent, to construct kinetic transition networks for the process of interest. The C-terminal domain (CTD) of the bacterial transcription factor RfaH provides an interesting example, where RfaH-CTD undergoes a dramatic all-α to all-β transition. In the all-α state RfaH-CTD interacts with the N-terminal domain (NTD) and functions as a regulator of transcription by masking the RNA polymerase binding site. However, upon dissociation from the NTD, the CTD refolds into the all-β state and aids in the activation of translation. Accordingly, this system provides a useful model for testing protein simulation techniques and for elucidating protein structural transitions in general. In this talk, I will discuss how the PEL approach can be used to compute the free energy surface and analyse the mechanics of (re)folding for the RfaH-CTD structural transition at atomistic resolution.

With faith and facts: Science and Biblical interpretation amongst Evangelical Christians in Brazil

Priscilla Garcia

This talk intends to address the role of science amongst Evangelical believers in Brazil. My arguments will be based on my 15 months of ethnographic fieldwork amongst Brazilian Christians who read the Bible literally, but who also believed science and religion are not opposites, but rather can be reconciled (this view is fundamentally different from dichotomous views which understand faith to oppose the rationality of science and vice-versa). This presentation, more specifically, will examine the way in which these Evangelical Christians reconcile faith and science beyond the dichotomy faith/reason.

The World’s Hottest Superglue: Materials requirements for better sealing in jet engines

Megan McGregor

Gas turbines function by using a high-temperature high-pressure gas stream to do work. In an industry where fractional increases in efficiency equate to hundreds of thousands of pounds, preventing loss of gas from this stream is crucially important. This requires sealing between the moving turbine blades and the stationary casing of the turbine. Any sealing solution must not only increase sealing efficiency but must stand up to the ever-increasing temperatures and rotational speeds of turbines, whilst remaining light. This talk will explain current and new sealing systems in the high pressure turbines, and explore the materials requirements for such new systems.
Poster exhibitions

1. Generalisation of computational model of reactivity for sp2 C-H activation reactions
   Liwei Cao

2. Maximising and Stabilising Luminescence in Metal Halide Perovskite Device Structures
   Mojtaba Abdi-Jalebi

3. How do our buildings shape our comfort practices?
   Rihab Khalid

4. Key successful factors of digitally enabled construction projects
   Thayla Zomer

5. Synthesis and Characterisation of Metastable Ion Conductors
   Jack Hodkinson

6. Understanding Expectation Propagation through toy examples
   Siddharth Swaroop

7. Contactless Smartcard Distance-Bounding Protocol Security Analysis
   Dominic Celiano

8. Network Latency in Data Centres
   Diana A. Popescu

9. Genetic stability of the mitochondrial genome in iPSC reprogramming
   Jannat Ijaz

10. The Everett and Copenhagen interpretations of Quantum Physics: a comparison
    Sivapalan Chelvanithhilan