## **LCLU WP Summer internships Projects**

Please email admin@lclu.cam.ac.uk with any queries, or contact the supervisors directly about the projects. This project list will be frequently updated so check back regularly.

## 1. Did magnetite cause biological molecules to become "one-handed"?

Supervisors: Prof Nicholas Tosca and Prof Richard Harrison, Department of Earth Sciences

# Co-applicants: Clancy Jiang, Dept of Earth Sciences; S. Furkan Ozturk and Dimitar Sasselov, Harvard University

Homochirality, or the exclusive selection of one of two possible mirror-image forms of sugars, amino acids, nucleotides and their respective polymers, is a fundamental signature of all life on Earth. However, the origins of homochirality have persisted as a central problem in research related to life's origins. A recent hypothesis has suggested that the mineral magnetite could have provided a source of spin-polarized electrons which may have led to the enrichment of one chiral form of bimolecular building blocks at a critical point in the origins of life. However, the efficiency of this process depends on the physical properties (size, shape, magnetic structure) of magnetite. What environments on the early Earth could have generated magnetite with suitable properties to induce homochirality?

To test the hypothesis that magnetite may have played a key role in the origin of hoimochirality, the aim of this project will be to investigate prebiotically-relevant synthesis routes for magnetite on the early Earth, and how its physical and magnetic properties vary under different conditions. The methodology will involve magnetite synthesis from oxygen-free water under a range of conditions relevant to prebiotic environments using experimental facilities in the Aqueous Geochemistry Laboratory, and a range of materials characterization facilities in the Department of Earth Sciences. The magnetic properties of the synthetic magnetite will be characterized in the NanoPalaeoMagnetism Laboratory, and the results will be synthesized in the context of current constraints on the efficiency of inducing enantiomeric excess with spin-polarized electrons. We anticipate the results will carry important implications for the natural environments and conditions under which magnetite may have facilitated enantiomeric excess on the early Earth, providing new perspective on the origins of life.

## 2. Can you detect an Exoplanet for <£100?

## Supervisors: Dr. Clark Baker, Matthew Hooton, Cavendish Astrophysics

In this project, the student will investigate whether you can detect an exoplanet transit from Cambridge using equipment that costs £100 or less.

Initially, the student will be given a crash course in observational astronomy. Using this knowledge, they will build an exposure time calculator (ETC)/ observation simulator for the photometric observation of an exoplanet. This will give the intern a good grounding and understanding of observational exoplanet science.

Applying the tool that the student has built, they will investigate the number of exoplanet transits from the exoplanet archive that they could re-observe with a small (0.1-0.3m) aperture telescope.

Time permitting, the student will look to procure the best instrument they can (pre-owned telescope and detector) with their modest budget of  $\sim$ £100 and attempt to make one of the observations that they have simulated.

## 3. How to make a fossil - and interpret the results

### Supervisors: Prof Nick Butterfield, Department of Earth Sciences

Fossils provide the only direct record of the deep-time history of life on Earth, but the pathways to producing them are complex and rarely successful. At the same time, there is any number of abiotic processes that can generate biology-mimicking form – pseudofossils. This project will examine a remarkable assemblage of fossils and pseudofossils from the ~100 million-year-old (mid-Cretaceous) Cambridge Greensand, with an eye to understanding the circumstances responsible for their preservation/formation, and what that might tell us about the biological, environmental and geochemical nature of the Greensand seas.

In addition to being green and sandy, the Cambridge Greensand is famous for its abundance of phosphatic 'coprolites' and the basis of the world's first artificial fertilizer. Although not actually fossil faeces, the industrialized excavation of phosphate-rich horizons in the late 19th century yielded an enormous diversity of bona fide fossils – from single celled phytoplankton to sponges, molluscs, echinoderms, aquatic reptiles and dinosaurs – most of which were similarly preserved via a process of phosphate biomineralization. This project will zero in on a number of these fossils and fossil-like structures in order to understand the sequence of events leading to their formation, not least the interplay between the original biominerals (calcite, aragonite, silica, phosphate), their selective preservation/dissolution/replacement, and the background effects of contemporaneous biological and sedimentological reworking.

The day to day work will involve the production and analysis of multiple petrographic thin-sections of Cambridge Greensand body fossils, trace fossils (burrows and borings) and 'coprolites.' Most of the analytical work will be conducted with a petrographic microscope, though there may also be an opportunity for some electron microscopy. Serial sectioning and virtual reassembly of key specimens would also be a possibility. On a more creative level, the student would be encouraged to think about how the preserved

onstituents relate back to the once-living organisms and their post-mortem biogeochemical processing.

## 4: Impact of the first arthropods on the biosphere

## Supervisors: Dr Stephen Pates and Dr Emily Mitchell, Department of Zoology

Arthropods have dominated the animal world since they first appeared during the Cambrian Explosion half a billion years ago. They were critical for construction and maintenance of the animal dominated biological pump throughout this time through mixing of the water column, playing crucial roles in the early Palaeozoic carbon cycle just as they do in the modern. However, links between their wide array of morphologies and their hydrodynamic impact have not been quantified.

Computational fluid dynamics approaches to determine the hydrodynamic performance of an array of arthropod morphologies provide an excellent opportunity to link form and function in arthropods, while morphometric and geometric morphometric approaches facilitate comparisons between extant and extinct forms. For this research project, specimens of modern crustaceans in the Cambridge Museum of Zoology will be utilised to quantify links between form and function in arthropods, providing valuable information that will provide insights into how the early diversification of form in Cambrian arthropods facilitated different life modes. Three-dimensional models of specimens of modern crustaceans in the Cambridge Museum of Zoology collections will be constructed. Specimens will be chosen that vary in carapace shape, abdomen length, and other morphological features seen to greatly vary in Cambrian arthropods. The hydrodynamic performance of these models will be quantified using computational fluid dynamics analyses. A range of conditions will be considered, including varying flow speeds and distances from the seafloor, to understand how morphology links to hydrodynamics in different environments and for different life modes. The morphology of extant specimens will then be quantitatively compared to Cambrian arthropods (data gathered from the literature). This will allow inference of how the morphological variation in these Cambrian arthropods impacted their hydrodynamic performance. Thus, the suitability of different Cambrian arthropod morphologies for different modes of life in these early animal ecosystems will be revealed.

## 5: Highly Accurate Quantum Astrochemistry

## Supervisors: Prof Alex Thom, Department of Chemistry

How can we determine the chemical constituents of the stars and planets? Spectroscopy is the obvious answer, but surprisingly experimental data is not usually sufficient in all but the most common molecules.

Such projects as ExoMol (www.exomol.com) attempt to draw together this experimental data, but still have limited success. Computational electronic structure techniques should

be able to come to the rescue, but the generally available present-day methods do not have the power to predict to the sub-wavenumber accuracy required.

With these highly accurate spectra, the prospect of identifying previously unknown species in exoplanets, space, or even in solar atmospheres becomes feasible.

To predict vibrational spectra of a molecule, however, the potential energy surface (PES) of such molecules (as well as the dipole moments) is required in order to perform the quantum mechanical calculations on the nuclei in order to generate spectra. To achieve sub-wavenumber accuracy it has been shown[1] that very high-level coupled cluster methods are needed to calculate the PES of small diatomic molecules around equilibrium, and the determination of the full dissociation PES does not appear to have been attempted to this level of accuracy.

This project will combine approaches based on Machine Learning for representing potential energy surfaces with Coupled Cluster methods (using conventional deterministic codes as well as new highly-parallelizable stochastic codes) to the prediction of accurate spectra of small diatomic molecules, beginning with the highly experimentally studied carbon monoxide and its cation and comparison with experimental databases to determine what level of theory is required to reach sub-wavenumber accuracy.

The project will involve interfacing existing quantum chemistry software with custom in-house python codes for calculating vibrational spectra, and the ideal student will have some familiarity with python programming.

## 6. Geochemical Signals from the low-energy limit to life

#### Supervisor: Alexandra V. Turchyn, Department of Earth Sciences

## Co-applicants: David Hodell, Department of Earth Sciences, Harold Bradbury, University of British Columbia, Vancouver, Department of Earth, Ocean, and Atmospheric Sciences

Microbial life finds a way to live in sedimentary environments, where the energy gain from the oxidation of organic matter coupled to anaerobic electron acceptors is minimal. In theory there is a minimum energy yield needed for life, but we are constantly finding microbial populations and consortia that are beating this minimum threshold, and finding ways to survive in **low energy** deserts. The metabolisms are similar to those thought to be present early in Earth history, when the planet was electron dense and electron accepting materials were few and far between. These include methanogenic archaea, sulfate reducing bacteria, and iron reducing bacteria.

Studying these populations is often best done by measuring the geochemistry of the fluids and sediment in which they grow. Expedition 397 of the International Ocean Discovery Program (IODP) sampled sediments and interstitial (pore) water at four sites off the Iberian Margin (Hodell et al., 2023). Previously, we analysed samples from a site-survey cruise and IODP Site U1385, which showed that this area has a dynamic microbial biosphere, with a sulfate-methane transition zone in the upper 50 meters of sediment (even shallower in places) and an active iron and sulfur cycle. During IODP Expedition 397, we sampled the pore fluids and sediment from this expedition and

this project will analyse the sulfur and oxygen isotopic composition of the pore fluids, which tells us about microbial sulfate metabolism, and the sulfur isotopic composition of the disseminated pyrite, particularly across the sulfate-methane transition zone. We showed previously that this zone preserves anomalously 'heavy' pyrite due to iron release during methane oxidation. This heavy pyrite might be a geochemical signal that could be used to look for methane-iron coupling and will yield insight into the geochemical record of Early life on the planet.

The samples are currently in the Department of Earth Sciences. The student will precipitate the sulfate as barium sulfate and dry the samples, and prepare them for mass spectrometry, and then analyse the sulfur and oxygen isotopic composition of the pore fluid sulfate. The student will also do chemical digestions of the sediment and measure the sulfur isotopic composition of the pyrite. The data analysis will take about half the time for the project, leaving ample time for the student to work with the research group and understand and interpret the data.

### 7. The composition of hot rocky planets

Supervisior: Dr Oliver Shorttle, Institute of Astronomy and Department of Earth Sciences

#### Co-applicants: Olivier Namur, KU Leven, Belgium and Mikel Kama, UCL

Rocky planets like Earth grow from solids present in the protoplanetary disk. Material that is present as a gas is not easily able to accrete to a growing planet, and so elements such as C, H and S, that are thermodynamically favoured to exist as gases, are often found to be significantly lower in abundance in planets compared to their host star. This is important because these elements are essential for life, so it raises the question of how carbon, water and sulfur came to be present on Earth. We know that in the solar system there is a wide diversity in the abundance of these life-essential elements between rocky planets, with Mars being overall more-rich in these than Earth, and Mercury having a particular large complement of sulfur. In this project we will perform a calculation to understand whether there are circumstances under which elements such as C, H, and S can be dominantly in the solid phase, and so make a major contribution to a growing rocky planet. If such a regime of planet growth is found, then we will go on to consider the observational consequences of this in the context of exoplanets.

#### Objectives

1) To calculate the gas and solid compositions of material in the hot inner region of a protoplanetary disk.

2) To vary the conditions of this calculation to investigate whether there are circumstances under which the presence C, H, and S can occur significantly as solids in the disk.

3) To make predictions for exoplanet atmospheric observations in light of the calculations.

#### Methodology

We will use an existing thermodynamic equilibrium code to model solid-gas phase equilibria in the protoplanetary disk environment. Advice will be given on the range of conditions to explore with the calculations, and support provided on interpreting the results.