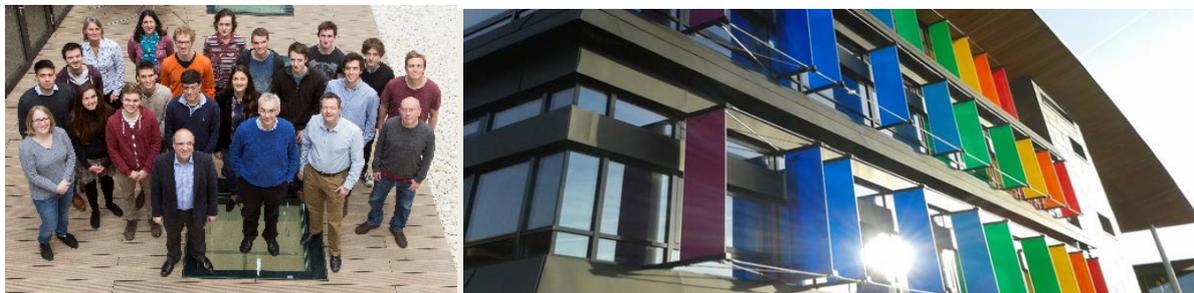


EPSRC CENTRE FOR DOCTORAL TRAINING IN COMPUTATIONAL METHODS FOR MATERIALS SCIENCE



BULLETIN ISSUE 6

Welcome to our sixth newsletter. We produce these twice a year to keep you informed of activities in our CDT. If you have suggestions for content or topics for future newsletters, please do send these to admin@csc.cam.ac.uk.

The main purpose of this edition of the newsletter is to introduce myself as the new Director of the CDT, and to welcome the students in our fourth cohort who started in October 2017. As incoming Director, I'd like to thank my predecessor, Professor Mike Payne, for his efforts in leading the CDT through its first phase of operation. He will be taking up a new position as Science Lead for the Cambridge Service for Data Driven Discovery (CSD3 - <https://www.csd3.cam.ac.uk/>), and we wish with him well with this effort. I look forward to working with all of you to continue this success, and most importantly to lead CDT through its first renewal bid, the call for which we expect to be published early in 2018.

As we enter the final two years of the first phase of CDT, it has been very encouraging to see how well the incoming cohort has bonded together. In the few months they have been here, they have been very busy with lectures - and there is plenty more to keep them busy for the rest of the academic year! Michaelmas term was heavy on lectures and computing practicals, and they are sitting mock exams before Christmas and "live" exams once they return from the Christmas break. We wish them all well with their studies, and you can find out more about their projects on pages 2 and 3.

Students in other cohorts have also been busy, with those in cohorts 1, 2 and 3 taking part in a Physics at Work exhibition demonstrating "Materials Modelling with Computers" to sixth form and high school students in September. Also, several students from cohort 1 took part in an internship to Biovia in October, where they carried out projects on molecular workings of battery electrolytes, chemical reaction dynamics, and a genetic algorithm for molecular design. Further details are given on page 4.

We are now recruiting our fifth cohort of students, so it is not too late to propose potential PhD projects to start in October 2018. If you, or any of your colleagues, would like to discuss possible PhD projects, want to find out more about the CDT or would like me to visit please feel free to get in contact with me at jae1001@cam.ac.uk.

James Elliott

Our 7 new CDT students in Year 4 cohort

	<p>Miriam Apsley</p> <p>I studied Natural Sciences at Cambridge up to Part II, following the Physics route, before switching to Maths for my Part III to take the fluids and astrophysics options. My Part III essay was on numerical simulation of magnetohydrodynamics (MHD).</p> <p>In my free time, I enjoy rowing and am currently trialling for the Cambridge university women's lightweight crew.</p>
	<p>Daniel Bennett</p> <p>I graduated from Trinity College Dublin with an undergraduate degree in theoretical physics this year. I am mainly interested in condensed matter theory, theoretical and mathematical physics. Last year I did two final year projects: one perturbation theory of quantum integrable spin chains, and one on <i>ab initio</i> simulations of high-entropy alloys.</p> <p>During my time at the CDT I will be studying under Professor Artacho. My project will involve studying the two-dimensional electron gas at the interface of thin film perovskites.</p>
	<p>Leon Devereux</p> <p>In June 2017, I graduated from Durham University with an MSci in Physics and Chemistry (within the Natural Sciences programme). In my final year, I used Density Functional Theory and time-dependent DFT in my research project to investigate the impact of ligand flexibility on optical properties of organometallic dyes. I also have some experience with molecular dynamics simulation of ion adsorption at solid-liquid interfaces (specifically the binding modes of glyphosate herbicide with clays).</p> <p>I am particularly interested in using computational chemistry methods combined with machine learning to inform design of new and improved dyes to be used in dye-sensitised solar cells, which I will work towards within the Molecular Engineering group supervised by Dr Jacqui Cole.</p>



Michael Hutcheon

I completed a combined undergraduate/masters degree in Physics at the university of Oxford, specialising in theoretical condensed matter physics. My masters research was on the use of low temperature superconducting systems in quantum computing, focusing on decoherence of charge qubits in such systems due to errant photons. My interest in computational physics partly stems from an internship at the Rutherford Appleton laboratory in computational high-energy physics.

I have joined the CDT with a hope to combine my interests in computational and condensed matter physics. I will be working with Professor Richard Needs in the theoretical condensed matter group.

In my spare time I enjoy writing and listening to music.



Mark Jenei

I graduated from UCL with a Master's Degree in Physics. In my Thesis project I was working on the sampling of the phase space of rigid two-dimensional molecules, adsorbed on an insulating surface. The project included choosing a suitable sampling method, which at the end I decided to be a type of Genetic Algorithm. In this CDT programme, I am going to work with Professor James Elliott. My main focus will be to investigate graph theoretical methods, combined with molecular modelling to understand polymerisation processes on multiple time-scales.



Haydn Lloyd

I graduated in 2017 from Cambridge, completing Part II and Part III in Chemistry, in which I studied methods to incorporate quantum statistics into molecular dynamics simulations.

I am now studying towards the MPhil and CDT in Computational Methods for Materials Science, where I will be studying non-linear vibrational spectroscopy of solid-aqueous interfaces, with Professor Sprik in the Chemistry department.

When I am not working on this, I am passionate about science communication and listening to heavy metal music.



Ben Shires

In 2017 I graduated from the University of Cambridge with a BA and MSci in Natural Sciences, specialising in Chemistry. My Part III project was supervised by Dr Alex Thom and involved the application of coupled-cluster based electronic structure techniques to small astronomical molecules with the aim to predict spectral properties.

I am now studying for an MPhil in Scientific Computing as part of the EPSRC CDT in computational methods for materials science at the University of Cambridge, with a PhD to follow. I will be supervised by Professor Chris Pickard of the Department of Materials Science and Metallurgy, as well as Professor Daan Frenkel of the Department of Chemistry. My project will focus on exploring energy landscapes and predicting crystal structures via energy minimisation. The aim is to develop the tools to predict how likely it is that a given structure will form from its building blocks and, more generally, how the probability to generate 'desirable' structures can be increased.

Physics at Work Exhibition



Delivering talk to high school students



Planning phase with Creativity@Home!

The first and second cohorts of the CDT took part in a series of talks entitled Physics at Work organised by the Cavendish Laboratory as part of their outreach program. These events had the intent of giving GCSE and A-Level students information about the research developed in this department.

Most of the first two cohorts of CDT CMMS participated, and were divided into groups of three to present a series of slides developed in a creativity workshop two weeks prior to the talks. The creativity workshop was facilitated by Amanda Scott from facilitateThis! Ltd. The workshop helped the students put together a presentation of the work developed by the CDT in a way which is appealing to middle to high school students. The presentation was divided into four thematic parts. These were given to smaller groups to conceptualise and create, and were later put together for the whole team to use.

The talks and workshop offered students the opportunity to develop their communication skills, particularly to a non-expert audience, as well as further team building and networking. We thank Professor James Elliott for the supervision throughout the event.

Tomé Magalhães Gouveia, CDT cohort 2

Visit of Cohort 1 to BIOVIA

The first cohort of the CDT spent a week in October participating in a placement with BIOVIA at the Cambridge Science Park. BIOVIA (a subsidiary of Dassault Systèmes) develops and licences research software for scientific applications as for example Materials Studio and CASTEP. The CDT-BIOVIA project was supervised by Dr Felix Hanke (a BIOVIA Senior Scientific Software Developer). During the placement, the students were split into three teams and were asked to focus on different research areas and provide daily feedback to the wider group.

Working in small groups was efficient and created an interesting dynamic. While the other groups worked on battery electrolytes and molecule screening, we worked on sensitivity analysis of chemical reaction networks. Here, we did not only learn about the scientific background but also about the standards of commercial software code.

This placement provided students with further opportunity for team building and networking allowing us to build on the foundations that were made during our previous years in the CDT.

Martin Schlegel, CDT cohort 1