EPSRC CENTRE FOR DOCTORAL TRAINING IN

COMPUTATIONAL METHODS FOR MATERIALS SCIENCE

BULLETIN ISSUE 5

Welcome to our fifth newsletter. We hope to 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 do send these to admin@csc.cam.ac.uk. The main purpose of this edition of the newsletter is to introduce the students in our third cohort who started in October 2016. It has been very encouraging to see how well this 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. They will sit mock exams before Christmas and "live" exams once they return from the Christmas break.

We are about to start recruiting our third cohort of students so it is not too late to propose potential PhD projects to start in October 2017. 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 mcp1@cam.ac.uk.

Mike Payne

Our 14 new CDT students in Year 3 cohort

Antonios Alvertis

I completed my undergraduate studies in Physics at the University of Athens in 2014, specialising in solid state physics and materials science. Being interested in the potential of organic materials for applications in solar cells and LEDs, I then followed the M.Sc. programme "Organic and Molecular Electronics" of the TU Dresden, where I performed research on their charge transport and emission properties.

It was the same interest that drove me towards becoming a member of the EPSRC CDT in Computational Methods for Materials Science, where I will be working with Dr. Alex Chin on singlet exciton fission in organic semiconductor materials – a promising phenomenon which leads to more efficient charge generation and will hopefully result in organic solar cells with a higher power conversion efficiency.

When I am not working on the above, I like to read and talk about the history of the Middle East, as well as to listen to the bouzouki and to rebetiko music.

Gareth Cornish

Having completed my undergraduate studies at the University of York, I have a strong background in theoretical and computational physics. My final year research project was titled "Molecular dynamics simulations of slurry targets", in which I used the LAMMPS molecular dynamics package to simulate shock compression of a solid-glue slurry. During the course of my previous studies, I also undertook a summer research project at Durham University, using CASTEP to perform geometry optimisations to determine muon stopping sites in solids.

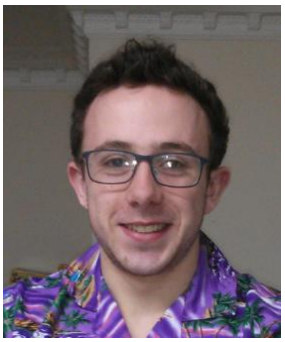
I am now reading towards the M.Phil. in Scientific Computing as part of the EPSRC CDT in Computational Methods for Materials Science at the University of Cambridge. During this and the following PhD programme I will be joining Prof Chris Pickard's Materials Theory Group in the Department of Materials Science and Metallurgy.

Callum Court

I am a new member of the Centre for scientific computing as a member of the EPSRC CDT in computational methods for materials science. My MPhil and PhD research will be undertaken within the Molecular Engineering group with a focus on using large scale data mining and machine learning to perform materials prediction, with a particular focus on predicting the properties of magnetic materials. Previously, I gained my MPhys degree in physics from Cardiff University. My masters research looked at simulating the dynamics of coupled qubit-resonator systems made from boron-doped diamond, by modelling the system with the Jaynes-Cummings model with the time-dependent Linblad master equation.

Luke Dicks

I graduated from Durham University with a Masters in Chemistry this summer after completing my final year project at a pharmaceutical company, where I used computational chemistry methods to build a workflow for estimating crystal habits. As part of the CDT I will continue to work within computational chemistry where I will be exploring the complex energy landscapes of biomolecules. The aim of my project is to use a knowledge of the underlying potential and free energy landscapes to probe protein coagulation pathways.



Stephen Farr

I have recently graduated with a MPhys in Physics from the University of Warwick. My final year research project was on non-stationary rare event sampling methods applied to molecular dynamics. My interest in computational physics is what led me to joining the CDT. I will be working in Dr Rosana Collepardo's group looking at determining chromatin structure of large scale (>100 nucleosome) arrays. I will be refining a coarse gain model which will incorporate unique experimental information. We aim to determine if, according to the experiments, nucleosomes within long chromatin fibers are packed orderly (e.g. forming super helical arrangements) or disorderly (e.g. adopting a molten-globule like organization) to pack the gene material within compact and de-condensed chromosomes.

Jessica Halliday

In 2015 I graduated from Cambridge with a BA and MSci in Natural Sciences, specialising in Materials Science. My Part III project focussed on molecular dynamics simulations of precipitation in Ni-base superalloys, using the LAMMPS molecular dynamics package. After a year spent working in financial consulting, I am currently studying for the MPhil in Scientific Computing as part of the CDT. I will be focussing on DFT simulations investigating electronic and nuclear stopping power.

James Klimavicz

I am a student in the MPhil in Scientific Computing as part of the CDT in Computational Methods for Material Science. Previously, I studied organic chemistry (BA, MS) and mathematics (BS) at Iowa State University, where I focused mainly on synthetic chemistry. With a substantial background in the maths and computer science, my current research interests lie in theoretical and computational chemistry. Using molecular mechanics and machine learning techniques, I hope to model energy landscapes of non-helical DNA conformers to improve the understanding of the formation and stability of these structures, which are caused by short, repeating nucleotide sequences folding in an atypical manner. These unusual conformations have been implicated in the formation of DNA replication errors, leading to genetic mutations.

Juraj Mavracic

My scientific interests include Theoretical and Computational Chemistry, as well as Computing in general.

I completed my Graduate Studies at the University of Vienna, where I was working on computational simulations of atomically thin layered solid state materials. To calculate optical and excitonic properties of these systems I used Density Functional Theory in combination with high level theoretical approaches, such as the GW method and the Bethe-Salpeter equation.

During my post graduate studies here in Cambridge I will work under the supervision of Prof. Stephen Elliott. My focus will be on phase-change memory materials, which are potential candidates for new logical devices enabling in-memory logic operations.

Here in Cambridge I don't miss any opportunity to attend interesting talks and lectures organised by the Scientific and Philosophical Societies. I enjoy inspiring discussions with my colleagues about specific problems or nature as a whole.

Jordan McKittrick

I am originally from Richmond, Virginia in the US. I studied biochemistry as an undergraduate at Columbia University in New York and then moved onto a master's in theoretical chemistry at Oxford, where I was a member of St Cross College. At Oxford I mostly worked on developing a mathematical method for handling stochastic processes with time-dependent drift and diffusion coefficients (i.e. very far from equilibrium).

At Cambridge, I am a member of Peterhouse. For the MPhil portion of the CDT, I intend to research co-translational protein folding using computer simulations in the chemistry department. I enjoy borrowing methods, ideas, and concepts from the physical sciences to answer questions in biology. In my free time I enjoy playing tennis.

Iria Pantazi

I am a CDT student studying for the MPhil in Scientific Computing with a PhD to follow. I will be working under the supervision of Dr Andrew Morris, and my research will concern the development of code for the study of lattice dynamics in carbon nanotubes.

I hold a diploma of Applied Sciences from National Technical University of Athens with specialization in Theoretical & Computational Physics, and Materials Science. My diploma thesis concerned the development of code in FORTRAN90, simulating light absorption in a device consisting of an optical diode, which enhanced light trapping mechanism, and graphene as the absorbing material.

In my free time I enjoy mountaineering.

Sundeep Popat

I have recently graduated with an MSci in Natural Sciences from University College London specialising in Physical Chemistry and Atomic Physics. My final year research project involved using global optimisation techniques such as genetic algorithms and data mining to search the potential energy surfaces of different sized TaAs nanoclusters for the lowest energy atomic configurations.

As part of the CDT I am currently taking several courses in scientific computing and atomistic modelling, after which, I will be joining the Althorpe group in Theoretical Chemistry. My research will build on recent advances in quantum simulation methods for treating liquid water. I will be using Matsubara Dynamics (a theory combining classical dynamics and quantum Boltzmann statistics) to develop new simulation methods for computing thermal time-correlation functions of liquid water using realistic model potential energy surfaces.

Eszter Szekely

I recently enrolled in the MPhil in Computational Methods for Materials Science as a part of the CDT. Previously, I completed a degree in Chemistry in Budapest, Hungary where I already conducted research in the field of molecular simulations. Here, I am going to join the research group of Gabor Csanyi where I will be developing state-of-the-art modelling technologies, such as machine learning combined with coupled cluster to describe mixtures of water with small molecules. The aim of this project is to describe compounds accurately without the computational cost of quantum chemistry methods. I am really interested in understanding material structure better and finding out more about the materials' inner nature: what makes them what they are, how the atomistic structures determine the macroscopic features.

Alexander Wade

I am currently studying for an MPhil in Scientific Computing having recently finished a MSci in Physics at King's College London. My interests are in the role of water at protein protein interfaces and the influence of water with respect to binding affinity and specificity. Water exists at protein interfaces, filling pockets when the protein surfaces do not conform perfectly or forming rings of water around binding hotspots. My main project will involve explicitly considering these waters in an effort to quantify their influence and improve protein design tools.

Nick Woods

My undergraduate studies consisted of an MPhys in Theoretical Physics from the University of York, and a MASt (Part III of the Mathematical Tripos) in Theoretical Physics and Applied Mathematics from the University of Cambridge. During my time at York, I specialised in computational condensed matter physics. My final year project involved investigating electronic properties of graphene nanostructures using quantum-derived models and CASTEP.

My work on the CDT is supervised jointly by Prof. Mike Payne and Dr. Phil Hasnip (York), and involves making algorithmic improvements to the density mixing schemes implemented in the self-consistent cycles of density functional theory software. Such improvements would not only increase the efficiency of density functional theory codes (allowing larger systems to be investigated), but could also converge the ground-state wavefunction for systems where the current schemes fail.