

*ab-initio molecular dynamics • phase-change memory materials •
thermoelectric materials • machine-learned interatomic potentials •
structure searching*

EDUCATION

- 2015– **PhD Chemistry**, *Chemical Physics Group*, University of Cambridge, *Expected submission 2018*.
2014–2015 **MPhil Scientific Computing**, University of Cambridge, *Distinction*.
2010–2014 **MSci Natural Sciences**, *Department of Chemistry*, University of Cambridge, *Upper Second Class (Hons)*.

RESEARCH

PhD **First and second principles simulations of Ge-Sb-Te phase-change memory materials**

with Prof. Stephen R. Elliott and Prof. Gábor Csányi (*University of Cambridge*)

Monte-Carlo sampling techniques for the fitting of a transferable Ge-Sb-Te machine-learned interatomic potential. Non-equilibrium molecular dynamics and stochastic-boundary conditions methods for calculating thermal conductivity. Structure searching and prediction of novel compositions for phase-change memory and thermoelectric materials. PhD research undertaken as a member of the EPSRC CDT for Computational Methods in Materials Science.

MPhil **Towards high-throughput simulation of Ge-Sb-Te phase change materials**

with Prof. Stephen R. Elliott and Prof. Gábor Csányi (*University of Cambridge*)

Worked on a machine-learned Gaussian Approximation Potential for the $\text{Ge}_2\text{Sb}_2\text{Te}_5$ phase-change memory material trained from *ab-initio* molecular dynamics trajectories and its application in large-scale and high-throughput simulations.

MSci ***Ab-initio* Molecular Dynamics of Phase Change Materials - NAND gate simulation**

with Dr. James Dixon and Prof. Stephen R. Elliott (*University of Cambridge*)

Worked on the *ab-initio* molecular-dynamics simulations of the atomistic effects of thermal pulse programming in the $\text{Ge}_2\text{Sb}_2\text{Te}_5$ phase-change memory material for applications in-memory logic and neuromorphic ("brain-like") computation.

UG **Synthesis and characterisation of functional cucurbituril-azobenzene host-guest assemblies**

summer student with Dr. Jesús del Barrio Lasheras and Prof. Oren Scherman (*University of Cambridge*)

INTERSHIPS

2012 **Rotatives Engineering Intern**

Cambridge Materials Placements for Undergraduates in Summer (CaMPUS) from the University of Cambridge Materials Science Department with Dr.-Ing. Hartmut Schlums (*Rolls-Royce Deutschland*) studying turbine blade lifetime in jet engines.

TEACHING

- 2016– Organiser of fortnightly simulation tutorials (*Chemical Physics Group*).
2017 Demonstrating Part IB Computational Practicals (*Department of Chemistry*).
2016 Demonstrating Part IA Labs (*Department of Chemistry*).
2016– Supervisor of Part II Theoretical Techniques course in Chemistry (Churchill College).
2015 Demonstrator IA C++ Computer Practicals (Engineering Laboratory).
2014–2016 Organiser of simulation sub-group meetings (*Chemical Physics Group*).

SIMULATION AND COMPUTING

DFT **VASP**, CP2K, CASTEP, GPAW

Platforms **Linux**

Languages **Python**, Julia, Fortran, C++

MD **LAMMPS**, QUIP

Packages **ASE**, quippy, pymatgen

Databases **MongoDB**, *SQL*

System administrator for the Elliott group *Hathor* computer cluster.

Tier-2 Resource Allocation (Project T2-CS020 "Thermoelectric Properties of Disordered Materials"): awarded 4 million CPU hours on the CSD3 supercomputer with Yuchen Hu and Prof. Stephen R. Elliott.

PUBLICATIONS

Status: in preparation, [submitted](#), [preprint](#), published.

3. Mocanu, F. C. *et al.* Modeling the Phase-Change Memory Material , $\text{Ge}_2\text{Sb}_2\text{Te}_5$, with a Machine-Learned Interatomic Potential. *The Journal of Physical Chemistry B* (2018).
2. Mavračić, J., **Mocanu, Felix C.**, Deringer, V. L., Csányi, G. & Elliott, S. R. Similarity Between Amorphous and Crystalline Phases: The Case of TiO_2 . *The Journal of Physical Chemistry Letters* **9**, 2985–2990. ISSN: 1948-7185 (June 2018).
1. Konstantinou, K., Lee, T. H., **Mocanu, Felix C.** & Elliott, S. R. Origin of radiation tolerance in amorphous $\text{Ge}_2\text{Sb}_2\text{Te}_5$ phase-change random-access memory material. *Proceedings of the National Academy of Sciences of the United States of America* **115**, 5353–5358. ISSN: 1091-6490 (May 2018).

CONFERENCE PRESENTATIONS

International Symposium on Doped Amorphous Chalcogenides and Devices

- 2018 Computer simulations of phase-change materials, Poster Presentation, Grasmere, United Kingdom - *Runner-up Prize*

European Phase-Change and Ovonic Symposium

- 2017 A machine-learned interatomic potential for Ge—Sb—Te phase-change materials, Poster Presentation, RWTH Aachen, Germany

Psi-k Conference on Electronic Structure

- 2015 A Gaussian Approximation Potential (GAP) for the $\text{Ge}_2\text{Sb}_2\text{Te}_5$ phase change material, Poster Presentation, San Sebastián, Spain

REFEREES

Prof. Stephen R. Elliott, University of Cambridge; sre1@cam.ac.uk

Prof Gábor Csányi, University of Cambridge; gc121@cam.ac.uk