Felix-Cosmin Mocanu

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fcmocanu

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 $Ge_2Sb_2Te_5$ phase-change memory material trained from *ab-initio* molecular dynamics trajectories and its application in large-scale and high-throughput simulations.

MSci ***Ab-inito* 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 $Ge_2Sb_2Te_5$ phase-change memory material for applications in-memory logic and neuromorphic ("brain-like") computation.

UG **Synthesis and characterisation of functional curcubituril-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	MD	**LAMMPS**, QUIP
Platforms	**Linux**	Packages	**ASE**, quippy, pymatgen
Languages	**Python**, Julia, Fortran, C++	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.

1. Konstantinou, K., Lee, T. H., **Mocanu, Felix C.** & Elliott, S. R. Origin of radiation tolerance in amorphous $Ge_2Sb_2Te_5$ 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).
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).

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 Ovonics 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 $Ge_2Sb_2Te_5$ 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