Edward Linscott

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Summary

I am currently a postdoctoral researcher at EPFL in the group of Prof. Nicola Marzari. Career highlights thus far include...

– Successful undergraduate studies culminating in receiving (a) the *Prince of Wales Award* for the most outstanding student completing an undergraduate degree at the University of Otago, and (b) the *Cambridge-Rutherford Memorial Scholarship* to enable doctoral studies at the University of Cambridge.

– Completing a masters and PhD at the University of Cambridge, during which I developed methods and code associated with DFT+U and dynamical mean field theory. This work has continued during my postdoc with the development of the BLOR functional and a high-throughput study of Hubbard and Hunds parameters.

– Developing and releasing the koopmans code, a package that implements Koopmans functionals. I am the lead author of this code. The "Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response" in late 2022 covered the use of this code, and had over 200 attendees.

– Supervising Yannick Schubert for his master's project and thesis. He said that "thanks to (Edward's) good choice of topics and guidance... achieving good results felt easy. Working with (Edward) was very motivating and a perfect start to a scientific career".

Broadly, my research investigates how we can improve the performance of density functional theory (DFT). Taking inspiration from known properties of the exact functional and our knowledge of the systemic errors of DFT, I (and others) have shown how we can construct inexpensive corrections to DFT that drastically improve its performance.

I am now looking for further opportunities where I can apply my expertise in density functional approximation development and my coding skills to develop the next generation of state-of-the-art methods for computational quantum chemistry and materials science.

Research and Education

École polytechnique fédérale de Lausanne
Switzerland

Postdoctoral researcher (1 Nov 2019 – present)

Supervisor: Prof. Nicola Marzari

The goal of my current postdoc is to drive the ongoing development of Koopmans functionals. To this end, I have been one of the main developers of the koopmans code, a package that (a) implements Koopmans functionals in `Quantum ESPRESSO` and (b) automates the various workflows that these functionals require. I also was involved in the development of the BLOR functional, a DFT+U-type corrective functional that enforeces the flat plane condition on localized subspaces, dispensing with the need for an ad hoc derivation from the Hubbard model.

University of Cambridge
United Kingdom

PhD in Physics (1 Oct 2015 – 26 Oct 2019)

Title: "Describing Correlation Effects in Biological Systems"

Supervisors: Prof. Mike Payne and Dr. Daniel Cole (Newcastle)

Funding: Cambridge-Rutherford Memorial Scholarship (valued at approx. €150,000; competitively awarded)

I developed novel approaches within linear-response theory for determining Hubbard and Hund's parameters from first principles for DFT + U calculations. I also developed a dynamical mean-field theory module for the linear scaling package ONETEP. I applied these tools to study (a) photodissociation of carboxy-heme (b) the electronic structure of hemocyanin, and (c) water-to-oxygen conversion performed by the oxygen evolving complex.

MPhil in Scientific Computing (1 Oct 2014 – 30 Sep 2015)

Title: "Strong Correlation Effects in the Electronic Structure of the Photosystem II Complex"

Supervisors: Prof. Mike Payne and Dr. Daniel Cole

Funding: EPSRC (valued at approx. €50,000)

Designed to lead into my PhD, my masters project motivated the need for models of the oxygen-evolving complex (OEC) that are thousands of atoms in size, and demonstrated that such calculations are feasible with the linear scaling density functional theory code ONETEP. The thesis also explored the DFT + U as a method for treating the correlation present in the OEC core.

University of Otago
New Zealand

Research Assistant (1 Mar 2014 – 31 July 2014)

Supervisor: Prof. P. Blair Blakie

I was briefly employed as a Research Assistant at the University of Otago, where I continued the work from my honours year studying the behaviour of quasi-2D dipolar Bose-Einstein condensates (BECs). This work resulted in a publication where we predicted an instability of dipolar BECs in regions of experimental interest.

BSc (Hons) in Physics (25 Feb 2013 – 4 Nov 2013)

Title: "Non-zero Temperature Theory for Ultra-Cold Dipolar Bose Gases"

Supervisor: Prof. P. Blair Blakie

This one-year honours programme was comprised of taught courses in physics and mathematics, and a research project exploring the effects of temperature on the stability of dipolar BECs. I graduated with first-class honours.

University of California, Berkeley
United States of America

Exchange (16 Aug 2012 – 14 Dec 2012)

I spent the final semester of my BSc (see below) on exchange at Berkeley.

University of Otago
New Zealand

BSc in Mathematics and Physics (1 Mar 2010 – 10 Nov 2012)

A three-year Bachelor's degree with a double-major in mathematics and physics. I obtained straight A^+ grades throughout.

Summer studentship (21 Nov 2011 – 30 Jan 2012)

A ten-week studentship in an interdisciplinary research group developing new computed tomography (CT) scanning technology. I wrote code to quantify the quality of their scans.

Skills

Programming

Used daily	Python, Fortran, Bash
Used monthly	MPI, OpenMP
Some experience	C++, MATLAB, CUDA

I developed koopmans, an open-source package for performing Koopmans functional calculations. I am a contributor to ONETEP, a commercially available scientific DFT code, and I am a developer of TOSCAM, a publically available DMFT code.

In addition to my formal training in scientific computing, during my PhD I sat in on *Machine Learning and Algorithims for Data Mining*, a master's course on machine learning run by the Department of Computer Science and Technology at the University of Cambridge.

I have participated in coding competitions such as Google Hash Code, Project Euler, and CodinGame.

Packages and software

Used daily	vscode, Quantum ESPRESSO, ASE, vim, LaTeX, SLURM, git
Used monthly	PyMol, VMD, ONETEP, TOSCAM, VESTA, spglib
Some experience	CASTEP, Siesta, Maestro

Teaching

2021-22	Lab demonstrator for master's course in atomistic and quantum simulation of materials	EPFL
2017	Supervised ten third-year students for thermal and statistical physics	University of Cambridge
2016	Supervised nine second-year students for experimental methods, oscillations, waves, optics, quantum mechanics, and condensed matter	University of Cambridge
2015	Supervised nine first-year students for physics	University of Cambridge
2013	Lab demonstrator, university tutor, and private tutor for first-year biological physics	University of Otago

Supervision and mentoring

During my postdoc I have supervised the Masters project and dissertation of Yannick Schubert. He said that "thanks to (Edward's) good choice of topics and guidance... achieving good results felt easy. Working with (Edward) was very motivating and a perfect start to a scientific career."

I also helped Hovan Lee (PhD student from King's College London) with his DMFT calculations on transferrin. A paper resulted from this work, of which I am the last author.

During the course of my PhD I provided support to two students. I spent a significant amount of time with M. A. Al-Badri (Masters, and then PhD student from King's College London), teaching him about DMFT and working with him on DMFT calculations on hemocyanin. I have hosted him in Cambridge twice, and visited him at KCL periodically. A paper resulted from this work. I was also the local port-of-call for S. Mansur (PhD student, Cambridge) for support running ONETEP calculations. This work has resulted in two publications.

Outreach

I assisted in Information Days at EPFL, introducing high school students to computational materials science research

I gave talks on computational physics to high school groups in the outreach event *Physics at Work 2017* at the Cavendish Laboratory.

Publications

A. Burgess, EBL, D. D. O'Regan, *A DFT+U type functional derived to explicitly address the flat plane condition*. arXiv:2210.17404 (2022)

G. C. Moore, M. K. Horton, A. M. Ganose, M. Siron, EBL, D. D. O'Regan, K. A. Persson, *High-throughput determination of Hubbard U and Hund J values for transition metal oxides via linear response formalism*. arXiv:2201.04213 (2022)

N. Colonna, R. De Gennaro, EBL, and N. Marzari, *Koopmans spectral functionals in periodic-boundary conditions*. J. Chem. Theory Comput. 18 (2022)

R. De Gennaro, N. Colonna, EBL, and N. Marzari, *Bloch's theorem in orbital-density-dependent functionals: Band structures from Koopmans spectral functionals*. Phys. Rev. B 106 (2022)

H. Lee, C. Weber, and EBL, *Many-body study of Iron (III)-bound human serum transferrin*. J. Phys. Chem. Lett. 13 (2022)

R. Kobayashi, T P. M. Goumans, N. Ole Carstensen, T. M. Soini, N. Marzari, I. Timrov, S. Poncé, EBL, C. J. Sewell, G. Pizzi, F. Ramirez, M. Bercx, S. P. . Huber, C. S. Adorf, and L. Talirz, *Virtual computational chemistry teaching laboratories – hands-on at a distance* J. Chem. Educ. 98 (2021)

EBL, D. J. Cole, N. D. M. Hine, M. C. Payne, and C. Weber, *ONETEP + TOSCAM: uniting dynamical mean field theory and linear-scaling density functional theory* J. Chem. Theory Comput. 16 (2020)

S. M. Masur, EBL, and C. J. Edgcombe, *Modelling a capped carbon nanotube by linear-scaling density-functional theory*, J. Electron Spectrosc. Relat. Phenom. 241 (2020) 146896

J. C. A. Prentice, J. Aarons, J. C. Womack, A. E. A. Allen, L. Andrinopoulos, L. Anton, R. A. Bell, A. Bhandari, G. A. Bramley, R. J. Charlton, R. J. Clements, D. J. Cole, G. Constantinescu, F. Corsetti, S. M-M. Dubois, K. K. B. Duff, J. María Escartín, A. Greco, Q. Hill, L. P. Lee, EBL, D. D. O'Regan, M. J. S. Phipps, L. E. Ratcliff, Á. Ruiz Serrano, E. W. Tait, G. Teobaldi, V. Vitale, N. Yeung, T. J. Zuehlsdorff, J. Dziedzic, P. D. Haynes, N. D. M. Hine, A. A. Mostofi, M. C. Payne, and C.-K. Skylaris, *The ONETEP linear-scaling density functional theory program*. J. Chem. Phys. 52 (2020) 174111

M. A. al-Badri, EBL, A. Georges, D. J. Cole, and C. Weber, *Superexchange mechanism and quantum many body excitations in the archetypal di-Cu oxo-bridge*. Comm. Phys. 3 (2020) 4

C. J. Edgcombe, S. M. Masur, EBL, J. Whaley-Baldwin, and C. H. W. Barnes, *Analysis of a capped carbon nanotube by linear-scaling density-functional theory*. Ultramicroscopy 198 (2019) 26

EBL, D. J. Cole, M. C. Payne, and D. D. O'Regan, *Role of spin in the calculation of Hubbard U and Hund's J parameters from first principles*. Phys. Rev. B 98 (2018) 235157

EBL and P. B. Blakie, *Thermally activated local collapse of a flattened dipolar condensate*. Phys. Rev. A 90 (2014) 053605

Grants and Scholarships

Year	Description	Approximate value
2018	EPSRC capital grant for computing hours on CSD3, a Tier-2 HPC centre	€30,000
2014	*LB Wood Scholarship* to supplement an existing scholarship for postgraduate study in Britain	€5,500
2013	*Cambridge–Rutherford Memorial Scholarship* for doctorate studies at the University of Cambridge	€150,000
	Douglass D. Crombie Award in Physics for an Otago graduate embarking on doctoral studies overseas	€4,000
2012	*University of Otago Prestige Scholarship in Science* to support honours study	€1,000
	Beverley Bursary for study towards physics honours (2011-2013)	€2,000
	The Alumni of the University of Otago in America Inc. Award to support an academic exchange to the United States	€600
2010	*Alumni Annual Appeal Scholarship* for study at the University of Otago	€4,000

	University of Otago Dux Scholarship for study at the University of Otago	€4,000
	University of Canterbury Dux Scholarship for study at the University of Canterbury (not taken up)	€4,000
	University of Canterbury Mathematics Scholarship for study at the University of Canterbury (not taken up)	€2,500
	University of Canterbury Science Scholarship for study at the University of Canterbury (not taken up)	€600

Awards and Prizes

2016	*Poster prize* at CCP9 Young Researchers' Event
2013	*Prince of Wales Award* for the most outstanding student completing an undergraduate degree at the University of Otago in 2013
2011	*Robert Jack / Institute of Physics Prize* for the top student in 200-level physics
	Gloria Olive Memorial Prize in Mathematics for the top student in 300-level mathematics
2010	*Department of Mathematics and Statistics Scholarship* for study at the University of Canterbury
	Robert Jack / Institute of Physics Prize for the top student in 100-level physics
	R. J. T. Bell Prize for the top student in 200-level mathematics
	New Zealand Institute of Chemistry Prize for the top student in CHEM111: Molecular Architecture

Conferences, Seminars, Schools, and Workshops

Year	Event	Location	Contribution
2022	Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response	Virtual	Invited talk; tutor
	9th Time-Dependent Density-Functional Theory Workshop: Prospects and Applications	Benasque	Invited talk
	DFT2022	Brussels	Contributed talk
	Psi-K conference	Lausanne	Poster
2021	ASE/Fireworks workshop on high-throughput workflows	Copenhagen	Poster
	Quantum Theory of Materials Seminar	Dublin	Invited talk
	APS March Meeting	Virtual	Contributed talk
	Virtual Winter School on Computational Chemistry	Virtual	Tutor
2020	Quantum Fluids in Isolation Seminar Series	Boston	Invited talk
2018	Autumn School on Correlated Electrons	Jülich	Poster
	CCP9 Young Researchers' Event	York	Poster
	DPG March Meeting	Berlin	
	CDT student-run seminar series	Cambridge	Invited talk
2017	Autumn School on Correlated Electrons	Jülich	Poster
	CCP-BioSim Conference: Frontiers of Biomolecular Simulation	Southampton	Poster
	New Generation in Strongly Correlated Electron Systems	Barcelona	Contributed talk
	ONETEP Masterclass	Warwick	Tutor
	Workshop on Localisation in Quantised Systems	London	

	CCP9 Young Researchers' Event	Cambridge	
2016	Physics by the Lake	Windsor	Poster
	CCP9 Young Researchers' Event	York	Poster
	"Programming: Modern Fortran" UCS workshop	Cambridge	
2015	Psi-K conference	San Sebastian	Poster
	ONETEP Masterclass	Cambridge	

Referees

	Prof. Mike Payne	**Prof. Nicola Marzari**
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