Edward Linscott

Nationality	New Zealander	*Email*	edward.linscott@epfl.ch
Date of birth	26/11/1991	*Phone*	+41 79 678 9641

Google Scholar · GitHub · Personal Website · Twitter

Summary

I am currently a postdoctoral researcher at EPFL in the group of Prof. Nicola Marzari. I am researching methods for improving 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 to construct inexpensive corrections to DFT that drastically improve its performance.

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

Career highlights thus far include...

– 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 Hund's 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" tutorial in late 2022 covered the use of this code, and had over 200 attendees.

– Supervising Yannick Schubert's 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".

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 enforces 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; LB Wood Scholarship; Douglass D. Crombie Award in Physics

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

Funding: University of Otago Prestige Scholarship in Science; Beverley Bursary

Awards: Prince of Wales Prize

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
Exchange (16 Aug 2012 – 14 Dec 2012)

Funding: The Alumni of the University of Otago in America Inc. Award

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)

Funding: University of Otago Dux Scholarship; Alumni Annual Appeal Scholarship

Awards: Robert Jack / Institute of Physics Prize; Gloria Olive Memorial Prize in Mathematics; R. J. T. Bell Prize; New Zealand Institute of Chemistry Prize

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

I am a confident programmer, with experience in various languages (including Python and Fortran) and implementing complex algorithms (primarily in the context of electronic structure calculations). I routinely employ good programming practices such as testing, documentation, and CI/CD.

Using these skills, 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 voluntarily attended *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 also enjoy coding competitions such as Google Hash Code, Project Euler, and CodinGame.

Languages and interfaces

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

Packages and software

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

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 and tutor for first-year biological physics	University of Otago

Supervision and mentoring

During my postdoc I supervised Yannick Schubert, a master's student. 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." One preprint has resulted from this work (with a second in preparation).

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 resulted in two publications.

Grant writing

I have written and received several grants (e.g. I was awarded an EPSRC capital grant for over 30K EUR of computing hours). I have also assisted with writing grant applications (e.g. a Swiss National Science Foundation grant that was awarded approximately 1M EUR and ranked in the top category of all applications).

Outreach

I have assisted at several information days at both EPFL and Cambridge, introducing high school students to computational materials science research.

Selected talks

Year	Event	Location	Contribution
2022	Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response	Virtual	Invited talk (video); Tutorial (video)
	9th Time-Dependent Density-Functional Theory Workshop: Prospects and Applications	Benasque	Invited talk
2021	Quantum Theory of Materials Seminar	Dublin	Invited talk (video)
2020	Quantum Fluids in Isolation Seminar Series	Boston	Invited talk (video)

Referees

	Prof. Mike Payne	**Prof. Nicola Marzari**
Address	Room 528, Mott Building	MED 2 1126
	Cavendish Laboratory	STI IMX THEOS
	University of Cambridge	École polytechnique fédérale de Lausanne
	19 J J Thomson Avenue	Route Cantonale
	Cambridge CB3 0HE	1015 Lausanne
	United Kingdom	Switzerland
Email	mcp1@cam.ac.uk	nicola.marzari@epfl.ch
Phone	+44 (0)1223 337254	+41 (0)21 693 1129

Publications

Y. Schubert, N. Marzari, and **EBL**, *Testing Koopmans spectral functionals on the analytically-solvable Hooke's atom*. arXiv:2212.05950 (2022)

A. Burgess, **EBL**, and 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, and 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