Curriculum Vitae

Name	Edward Baxter Linscott		
Nationality	New Zealander	*Email*	edward.linscott@epfl.ch
Date of birth	26/11/1991	*Website*	elinscott.github.io

Research overview

Broadly, I am interested in how we can improve the performance of density functional theory (DFT). Inspired by known properties of the exact functional and the systemic errors of DFT, one can construct inexpensive corrections to DFT that drastically improve its performance.
Most recently, I have developed the `koopmans` code, a package that implements Koopmans functionals. By imposing a generalized piecewise energy condition, these functionals obtain spectral properties with comparable accuracy to GW at a fraction of the cost.
I am now looking for opportunities to extend this line of research, both by continuing to push theoretical and computational developments, and by capitalizing on our existing theories to study systems of scientific interest (e.g. novel photovoltaics).

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.

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)

Many key reactions in biology are performed by metalloproteins. These systems are a challenge to accurately simulate due to two contrasting reasons. Firstly, the strong correlation present due to the transition metal atoms requires more accurate theories than semi-local DFT. And secondly the ambient protein environment requires explicit treatment of thousands of atoms at the quantum-mechanical level. Over the course of my PhD 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 dipolar Bose gases. 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 comprised of taught courses in physics and mathematics, and a research project. My research project explored the effects of temperature on the behaviour of quasi-2D dipolar Bose-Einstein condensates; that is, BECs whose atoms (a) interact with an appreciable magnetic dipole-dipole moment and (b) are contained within a 2D optical trap. 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)

During my undergraduate studies I spent a summer in a studentship with a interdisciplinary research group developing new computed tomography (CT) scanning technology. I was involved in developing software that allowed the research team to quantify the quality of their images (and hence assess the performance of their machines during development).

Publications

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)	1 citation
H. Lee, C. Weber, and EBL, *Many-body study of Iron (III)-bound human serum transferrin*. J. Phys. Chem. Lett. 13 (2022)	
N. Colonna, R. De Gennaro, EBL, and N. Marzari, *Koopmans spectral functionals in periodic-boundary conditions* arXiv:2202.08155 (2021)	
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)	8 citations
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)	5 citations

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	3 citations
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	73 citations
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	7 citations
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	14 citations
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	33 citations
EBL and P. B. Blakie, *Thermally activated local collapse of a flattened dipolar condensate*. Phys. Rev. A 90 (2014) 053605	9 citations; selected as an Editors' Suggestion

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
2021	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	

Skills

Programming

Used daily	Fortran, Python, 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 2017 I audited *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 participated in Google Hash Code 2018. I sporadically compete on Project Euler and CodinGame

Packages and Software

Used daily	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

Mentoring

During my postdoc I have supervised the Masters project and dissertation of Yannick Schubert.

I also helped Hovan Lee (PhD student from King's College London) with his DMFT calculations on transferrin. A paper resulted from this work, for 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 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 gave talks on computational physics to high school groups in the outreach event *Physics at Work 2017* at the Cavendish Laboratory.

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