

Curriculum Vitae

<i>Name</i>	Edward Baxter Linscott		
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<i>Date of birth</i>	26/11/1991	<i>Website</i>	https://elinscott.github.io/

Professional Experience

start date	end date	job title	institution
1 Nov 2019	present	Postdoctoral Researcher	École polytechnique fédérale de Lausanne
I am currently a postdoc at EPFL, Lausanne, Switzerland, in the group of Prof. Nicola Marzari. I am working on developing Koopmans spectral functionals for addressing systematic errors in density functional theory.			
1 Mar 2014	31 July 2014	Research Assistant	University of Otago
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.			
21 Nov 2011	30 Jan 2012	Summer Studentship	University of Otago
I spent a summer in a studentship with an engineering/physics/medical 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).			

Education

start date	end date	degree/course	institution	grade
1 Oct 2015	26 Oct 2019	PhD in Physics	University of Cambridge	
<i>Title:</i> "Describing Correlation Effects in Biological Systems"				
<i>Supervisors:</i> Prof. Mike Payne and Dr. Daniel Cole (Newcastle)				
<i>Funding:</i> 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 density-functional theory. 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.				
1 Oct 2014	30 Sep 2015	MPhil in Scientific Computing	University of Cambridge	Distinction
<i>Title:</i> "Strong Correlation Effects in the Electronic Structure of the Photosystem II Complex"				
<i>Supervisors:</i> Prof. Mike Payne and Dr. Daniel Cole				
<i>Funding:</i> 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.				
25 Feb 2013	4 Nov 2013	BSc (Hons) in Physics	University of Otago	First Class
<i>Title:</i> "Non-zero Temperature Theory for Ultra-Cold Dipolar Bose Gases"				
<i>Supervisor:</i> 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. (See the "Professional Experience" section for the outcome of this research.)

1 Mar 2010	10 Nov 2012	BSc in Mathematics and Physics	University of Otago and University of California Berkeley	Straight A+'s
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A three-year Bachelor's degree with a double-major in mathematics and physics. I spent the final semester of this degree on exchange at Berkeley.

Publications

R. De Gennaro, N. Colonna, EBL, and N. Marzari, <i>Bloch's theorem in orbital-density-dependent functionals: Band structures from Koopmans spectral functionals</i> . Phys. Rev. B 106 (2022)	1 citation
H. Lee, C. Weber, and EBL, <i>Many-body study of Iron (III)-bound human serum transferrin</i> . J. Phys. Chem. Lett. 13 (2022)	
N. Colonna, R. De Gennaro, EBL, and N. Marzari, <i>Koopmans spectral functionals in periodic-boundary conditions</i> 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, <i>Virtual computational chemistry teaching laboratories – hands-on at a distance</i> J. Chem. Educ. 98 (2021)	8 citations
EBL, D. J. Cole, N. D. M. Hine, M. C. Payne, and C. Weber, <i>ONETEP + TOSCAM: uniting dynamical mean field theory and linear-scaling density functional theory</i> J. Chem. Theory Comput. 16 (2020)	5 citations
S. M. Masur, EBL, and C. J. Edgcombe, <i>Modelling a capped carbon nanotube by linear-scaling density-functional theory</i> , 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, <i>The ONETEP linear-scaling density functional theory program</i> . J. Chem. Phys. 52 (2020) 174111	73 citations
M. A. al-Badri, EBL, A. Georges, D. J. Cole, and C. Weber, <i>Superexchange mechanism and quantum many body excitations in the archetypal di-Cu oxo-bridge</i> . Comm. Phys. 3 (2020) 4	7 citations
C. J. Edgcombe, S. M. Masur, EBL, J. Whaley-Baldwin, and C. H. W. Barnes, <i>Analysis of a capped carbon nanotube by linear-scaling density-functional theory</i> . Ultramicroscopy 198 (2019) 26	14 citations
EBL, D. J. Cole, M. C. Payne, and D. D. O'Regan, <i>Role of spin in the calculation of Hubbard U and Hund's J parameters from first principles</i> . Phys. Rev. B 98 (2018) 235157	33 citations
EBL and P. B. Blakie, <i>Thermally activated local collapse of a flattened dipolar condensate</i> . 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	<i>LB Wood Scholarship</i> to supplement an existing scholarship for postgraduate study in Britain	€5,500
2013	<i>Cambridge–Rutherford Memorial Scholarship</i> for doctorate studies at the University of Cambridge	€150,000
	<i>Douglass D. Crombie Award in Physics</i> for an Otago graduate embarking on doctoral studies overseas	€4,000
2012	<i>University of Otago Prestige Scholarship in Science</i> to support honours study	€1,000
	<i>Beverley Bursary</i> for study towards physics honours (2011-2013)	€2,000
	<i>The Alumni of the University of Otago in America Inc. Award</i> to support an academic exchange to the United States	€600
2010	<i>Alumni Annual Appeal Scholarship</i> for study at the University of Otago	€4,000
	<i>University of Otago Dux Scholarship</i> for study at the University of Otago	€4,000
	<i>University of Canterbury Dux Scholarship</i> for study at the University of Canterbury (not taken up)	€4,000
	<i>University of Canterbury Mathematics Scholarship</i> for study at the University of Canterbury (not taken up)	€2,500
	<i>University of Canterbury Science Scholarship</i> for study at the University of Canterbury (not taken up)	€600

Awards and Prizes	
2016	<i>Poster prize</i> at CCP9 Young Researchers' Event
2013	<i>Prince of Wales Award</i> for the most outstanding student completing an undergraduate degree at the University of Otago in 2013
2011	<i>Robert Jack / Institute of Physics Prize</i> for the top student in 200-level physics
	<i>Gloria Olive Memorial Prize in Mathematics</i> for the top student in 300-level mathematics
2010	<i>Department of Mathematics and Statistics Scholarship</i> for study at the University of Canterbury
	<i>Robert Jack / Institute of Physics Prize</i> for the top student in 100-level physics
	<i>R. J. T. Bell Prize</i> for the top student in 200-level mathematics
	<i>New Zealand Institute of Chemistry Prize</i> 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 am a contributor to ONETEP , a commercially available scientific DFT code, and a developer of TOSCAM, a publically available DMFT code		
In 2017 I audited Machine Learning and Algorithms 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, L ^A T _E X, SLURM, git	
Used monthly	PyMol, VMD, ONETEP, TOSCAM,	
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.

Interests

I am a violinist, and have been a member (and concertmaster) of many orchestras including the New Zealand Symphony Secondary Schools Orchestra, the Christchurch Youth Orchestra, and the Cambridge Musical Society Symphony Orchestra. I love the outdoors and am an avid runner, cyclist, camper, and hiker.

Referees		
	Prof. Mike Payne	Prof. P. Blair Blakie
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