Dr. Edward **Linscott**

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Researcher seeking to create the next generation of state-of-the-art methods for computational spectroscopy

Summary

I am a postdoctoral researcher at the Paul Scherrer Institute in the group of Prof. Nicola Marzari, researching methods to improve density functional theory (DFT). Taking inspiration from the properties of the exact functional and DFT's systematic errors, I (and others) have shown how to construct inexpensive corrections that drastically improve DFT's performance.

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.
- Designing, developing, and releasing the koopmans code, a package that implements Koopmans functionals. I am the lead author of this code. The code has attracted wide interest: an online tutorial had over 200 attendees; it is being used by industrial partners.
- 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

Postdoctoral researcher
PAUL SCHERRER INSTITUTE
Nov 2023 – present
Villigen, Switzerland

The goal of my current postdoc is to accurately predict and interpret experimental spectroscopies, such as ARPES spectra. To this end, I am continuing to develop Koopmans functionals and the associated koopmans code. I am working to make these powerful computational tools accessible and user-friendly for experimental colleagues.

Postdoctoral researcher
ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE
Nov 2019 – Oct 2023
Lausanne, Switzerland

I drove the ongoing development of Koopmans functionals. To this end, I developed 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 DFT+*U*-type functionals that dispense with the need for an *ad hoc* derivation from the Hubbard model.

PhD in Physics
UNIVERSITY OF CAMBRIDGE
Oct 2015 – Sep 2019
Cambridge, UK

Thesis Describing Correlation Effects in Biological Systems | *Supervisors* Prof. Mike Payne and Dr. Daniel Cole

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) the oxygen-evolving complex.

MPhil in Scientific Computing
UNIVERSITY OF CAMBRIDGE
Oct 2014 – Sep 2015
Cambridge, UK

Thesis Strong Correlation Effects in the Electronic Structure of the Photosystem II Complex
Supervisors Prof. Mike Payne and Dr. Daniel Cole

My masters thesis motivated the need for models of the oxygen-evolving complex (OEC) that are thousands of atoms in size, demonstrated that such calculations are feasible with linear-scaling DFT, and explored DFT+*U* as a method for treating correlation present in the OEC.

Research Assistant
UNIVERSITY OF OTAGO
Mar – Jul 2014
Dunedin, New Zealand

I studied 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
UNIVERSITY OF OTAGO
Mar 2010 – Nov 2013
Dunedin, New Zealand

Thesis Non-zero Temperature Theory for Ultra-Cold Dipolar Bose Gases | *Supervisor* Prof. P. Blair Blakie

This four-year honours programme comprised of taught courses (mostly in physics and mathematics) and a final-year research project exploring the effects of temperature on the stability of dipolar BECs. In my third year I spent a semester abroad at the University of California, Berkeley. I graduated with first-class honours and a straight A+ record.

Selected Prizes and Awards

award	*description*	*value (NZD)*	*year*
Cambridge-Rutherford Memorial Scholarship	to support doctoral study at the University of Cambridge	approx 275,000	2013
Prince of Wales Award	for the most outstanding student completing an undergraduate degree at the University of Otago	500	2013
LB Wood Travelling Scholarship	to support overseas doctoral studies	9,000	2014
Douglass D. Crombie Award in Physics	to support postgraduate research in physics	7,000	2013
University of Otago Prestige Scholarship in Science	for undergraduate academic achievement	1,500	2012

Skills

Programming

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

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

In addition to my formal training in scientific computing, I voluntarily attended Machine Learning and Algorithims for Data Mining, a master's course on machine learning. I also enjoy coding competitions such as Google Hash Code, Project Euler, and CodinGame.

Languages and interfaces		**Packages and software**	
Used daily	Python, Fortran, Bash	*Used daily*	vim, git, vscode, Quantum ESPRESSO, ASE, LaTeX, SLURM
Some experience	C++, MPI, OpenMP, MATLAB, CUDA	*Extensive experience*	scikit-learn, pandas, ONETEP, PyMol, typst
		Some experience	CASTEP, Siesta, Maestro, VMD, LAMMPS, spglib, VESTA, Blender

Teaching

role	*course*	*level*	*institution*	*number of students*	*contact hours*	*year(s)*
Lab demonstrator	Atomistic and quantum simulation of materials	master's	EPFL	two-on-30 (approx)	2/week for 3 weeks	2021–23
Supervisor	Thermal and statistical physics	third-year	Cambridge	one-on-three or -four	3/week for 12 weeks	2017
Supervisor	Exp. methods, oscillations, waves, optics, quantum mech., and condensed matter	second-year	Cambridge	one-on-three	3/week for 36 weeks	2016
Supervisor	Physics	first year	Cambridge	one-on-three	3/week for 36 weeks	2015
Lab demonstrator	Biological physics	first-year	Otago	six-on-100 (approx)	6/week for 13 weeks	2013

Supervision and mentoring

I am currently co-supervising Marija Stojkovic (PhD; EPFL; 2021–present).

I supervised Yannick Schubert (Masters; ETHZ; 2021–22). 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." Two papers resulted from this work.

While not formally being their supervisor, I also helped…

- F. Haddadi (PhD; EPFL) with DFT+*U*+*J* calculations; a paper resulted from this work.
- H. Lee (PhD; King's College London) with DMFT calculations on transferrin; a paper resulted from this work, of which I am the last author.
- M. A. Al-Badri (Master's and PhD; King's College London) with DMFT calculations on hemocyanin; a paper resulted from this work.
- S. Mansur (PhD; Cambridge) with linear-scaling DFT calculations on carbon nanotubes; two papers resulted from this work.

Grant writing

I have written and received several grants (e.g. an EPSRC capital grant for over 50k NZD of computing hours). I have also assisted with writing grant applications (e.g. SNSF Grant 213082 awarded approx. 2M NZD and ranked in the top category of all applications).

Service and Outreach

- I have reviewed articles for *Phys. Rev. Lett.* and *Phys. Rev. B*
- I have helped run tutorials on koopmans 🎥, Quantum ESPRESSO, and ONETEP
- I am on the PhD committee of D. Tang (University of Zurich; 2023–present)
- I assisted at information days at EPFL and Cambridge, introducing high school students to computational materials science research

Selected Invited Talks

2025	Psi-k 2025 Conference	Lausanne, CH	
2024	Beyond ground state simulations: Navigating challenges in excited states of molecules and materials	Lausanne, CH	
2023	Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response	Pavia, IT	🎥
2022	Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response	virtual	🎥
	9th Time-Dependent Density-Functional Theory Workshop: Prospects and Applications	Benasque, ES	
2021	Quantum Theory of Materials Seminar	Dublin, IE	🎥
2020	Quantum Fluids in Isolation Seminar Series	virtual	🎥

Publications

1. Y. Schubert, S. Luber, N. Marzari, & E. Linscott. Predicting Electronic Screening for Fast Koopmans Spectral Functional Calculations. *npj Comput. Mater. (accepted)* (2024) 10.48550/arXiv.2406.15205
2. A. C. Burgess, E. Linscott, & D. D. O'Regan. Tilted-Plane Structure of the Energy of Finite Quantum Systems. *Physical Review Letters* 133, 26404 (2024) 10.1103/PhysRevLett.133.026404
3. J. E. Ingall, E. Linscott, N. Colonna, A. J. Page, & V. J. Keast. Accurate and Efficient Computation of the Fundamental Bandgap of the Vacancy-Ordered Double Perovskite Cs_2TiBr_6. *The Journal of Physical Chemistry C* 128, 9217–9228 (2024) 10.1021/acs.jpcc.3c07957
4. G. C. Moore, M. K. Horton, E. Linscott, A. M. Ganose, M. Siron, D. D. O'Regan, & K. A. Persson. High-Throughput Determination of Hubbard U and Hund J Values for Transition Metal Oxides via the Linear Response Formalism. *Physical Review Materials* 8, 14409 (2024) 10.1103/PhysRevMaterials.8.014409
5. F. Haddadi, E. Linscott, I. Timrov, N. Marzari, & M. Gibertini. On-Site and Intersite Hubbard Corrections in Magnetic Monolayers: The Case of $FePS_3$ and CrI_3. *Physical Review Materials* 8, 14007 (2024) 10.1103/PhysRevMaterials.8.014007
6. A. C. Burgess, E. Linscott, & D. D. O'Regan. The Convexity Condition of Density-Functional Theory. *The Journal of Chemical Physics* 159, 211102 (2023) 10.1063/5.0174159
7. E. B. Linscott, N. Colonna, R. De Gennaro, N. L. Nguyen, G. Borghi, A. Ferretti, I. Dabo, & N. Marzari. Koopmans: An Open-Source Package for Accurately and Efficiently Predicting Spectral Properties with Koopmans Functionals. *Journal of Chemical Theory and Computation* 19, 7097–7111 (2023) 10.1021/acs.jctc.3c00652
8. Y. Schubert, N. Marzari, & E. Linscott. Testing Koopmans Spectral Functionals on the Analytically Solvable Hooke's Atom. *The Journal of Chemical Physics* 158, 144113 (2023) 10.1063/5.0138610
9. A. C. Burgess, E. Linscott, & D. D. O'Regan. DFT+U-type Functional Derived to Explicitly Address the Flat Plane Condition. *Physical Review B* 107, L121115 (2023) 10.1103/PhysRevB.107.L121115
10. N. Colonna, R. De Gennaro, E. Linscott, & N. Marzari. Koopmans Spectral Functionals in Periodic Boundary Conditions. *Journal of Chemical Theory and Computation* 18, 5435–5448 (2022) 10.1021/acs.jctc.2c00161
11. R. De Gennaro, N. Colonna, E. Linscott, & N. Marzari. Bloch's Theorem in Orbital-Density-Dependent Functionals: Band Structures from Koopmans Spectral Functionals. *Physical Review B* 106, 35106 (2022) 10.1103/PhysRevB.106.035106
12. H. Lee, C. Weber, & E. B. Linscott. Many-Body Study of Iron(III)-Bound Human Serum Transferrin. *The Journal of Physical Chemistry Letters* 13, 4419–4425 (2022) 10.1021/acs.jpclett.2c00680
13. R. Kobayashi, T. P. M. Goumans, N. O. Carstensen, T. M. Soini, N. Marzari, I. Timrov, S. Poncé, E. B. Linscott, C. J. Sewell, G. Pizzi, F. Ramirez, M. Bercx, S. P. Huber, C. S. Adorf, & L. Talirz. Virtual Computational Chemistry Teaching Laboratories — Hands-on at a Distance. *Journal of Chemical Education* 98, 3163–3171 (2021) 10.1021/acs.jchemed.1c00655
14. E. B. Linscott, D. J. Cole, N. D. M. Hine, M. C. Payne, & C. Weber. ONETEP + TOSCAM: Uniting Dynamical Mean Field Theory and Linear-Scaling Density Functional Theory. *Journal of Chemical Theory and Computation* (2020) 10.1021/acs.jctc.0c00162
15. 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. M. Escartín, A. Greco, Q. Hill, L. P. Lee, E. Linscott, D. D. O'Regan, M. J. S. Phipps, L. E. Ratcliff, Á. R. 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, & C.-K. Skylaris. The ONETEP Linear-Scaling Density Functional Theory Program. *The Journal of Chemical Physics* 152, 174111 (2020) 10.1063/5.0004445
16. S. M. Masur, E. B. Linscott, & C. J. Edgcombe. Modelling a Capped Carbon Nanotube by Linear-Scaling Density-Functional Theory. *Journal of Electron Spectroscopy and Related Phenomena* 241, 146896 (2020) 10.1016/j.elspec.2019.146896
17. M. A. al- Badri, E. Linscott, A. Georges, D. J. Cole, & C. Weber. Superexchange Mechanism and Quantum Many Body Excitations in the Archetypal Di-Cu Oxo-Bridge. *Communications Physics* 3, 1–8 (2020) 10.1038/s42005-019-0270-1
18. C. Edgcombe, S. Masur, E. Linscott, J. Whaley-Baldwin, & C. Barnes. Analysis of a Capped Carbon Nanotube by Linear-Scaling Density-Functional Theory. *Ultramicroscopy* 198, (2019) 10.1016/j.ultramic.2018.11.007
19. E. B. Linscott, D. J. Cole, M. C. Payne, & D. D. O'Regan. Role of Spin in the Calculation of Hubbard U and Hund's J Parameters from First Principles. *Physical Review B* 98, 235157 (2018) 10.1103/PhysRevB.98.235157
20. E. B. Linscott & P. B. Blakie. Thermally Activated Local Collapse of a Flattened Dipolar Condensate. *Physical Review A* 90, 1–7 (2014) 10.1103/PhysRevA.90.053605

Referees

Prof. Nicola Marzari

Postdoc Supervisor, 2019 - present

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