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 — *2023 – present*
PAUL SCHERRER INSTITUTE — *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 — *2019 – 2023*
ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE — *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 — *2015 – 2019*
UNIVERSITY OF CAMBRIDGE — *Cambridge, UK*

Thesis Describing Correlation Effects in Biological Systems | *Supervisors* Prof. Mike Payne and Dr. Daniel Cole
Funding Cambridge-Rutherford Memorial Scholarship (valued at approx. 275k NZD; 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) the oxygen-evolving complex.

MPhil in Scientific Computing — *2014 – 2015*
UNIVERSITY OF CAMBRIDGE — *Cambridge, UK*

Thesis 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

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 — *2014*
UNIVERSITY OF OTAGO — *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 — *2010 – 2013*
UNIVERSITY OF OTAGO — *Dunedin, New Zealand*

Thesis 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 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.

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 was 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	scikit-learn, pandas, ONETEP, PyMol, typst
Some experience	CASTEP, Siesta, Maestro, VMD, LAMMPS, spglib, VESTA, Blender

Teaching

2021 - 2023	EPFL	Lab demonstrator for master's course in atomistic and quantum simulation of materials
2017	University of Cambridge	Supervised ten third-year students for thermal and statistical physics
2016	University of Cambridge	Supervised nine second-year students for experimental methods, oscillations, waves, optics, quantum mechanics, and condensed matter
2015	University of Cambridge	Supervised nine first-year students for physics
2013	University of Otago	Lab demonstrator and tutor for first-year biological physics

Supervision and mentoring

During my first 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 paper has resulted from this work (with a second under review).

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 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 resulted in two publications.

Grant writing

I have written and received several grants (e.g. I was awarded an EPSRC capital grant for over 50k NZD of computing hours). I have also assisted with writing grant applications (e.g. a Swiss National Science Foundation grant that was awarded approximately 2M NZD 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

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

Publications

1. Y. Schubert, S. Luber, N. Marzari & E. Linscott. Predicting Electronic Screening for Fast Koopmans Spectral Functional Calculations. (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. *Phys. Rev. Lett.* 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. *J. Phys. Chem. C* 128, 9217–9228 (2024) 10.1021/acs.jpcc.3c07957
4. G. C. Moore *et al.* High-Throughput Determination of Hubbard U and Hund J Values for Transition Metal Oxides via the Linear Response Formalism. *Phys. Rev. Mater.* 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. *Phys. Rev. Mater.* 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. *J. Chem. Phys.* 159, 211102 (2023) 10.1063/5.0174159
7. E. B. Linscott *et al.* Koopmans: An Open-Source Package for Accurately and Efficiently Predicting Spectral Properties with Koopmans Functionals. *J. Chem. Theory Comput.* 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. *J. Chem. Phys.* 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. *Phys. Rev. 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. *J. Chem. Theory Comput.* 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. *Phys. Rev. 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. *J. Phys. Chem. Lett.* 13, 4419–4425 (2022) 10.1021/acs.jpclett.2c00680
13. R. Kobayashi *et al.* Virtual Computational Chemistry Teaching Laboratories — Hands-on at a Distance. *J. Chem. Educ.* 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. *J. Chem. Theory Comput.* (2020) 10.1021/acs.jctc.0c00162
15. J. C. A. Prentice *et al.* The ONETEP Linear-Scaling Density Functional Theory Program. *J. Chem. Phys.* 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. *J. Electron Spectrosc. Relat. Phenom.* 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. *Commun. Phys.* 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. *Phys. Rev. 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. *Phys. Rev. A* 90, 1–7 (2014) 10.1103/PhysRevA.90.053605

Referees

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