

Hugh G. A. Burton

EMPLOYMENT

10/2020 – Present	Astor Junior Research Fellow in Chemistry New College, Oxford, UK Visiting Researcher Department of Chemistry, University of Oxford, Oxford, UK
04/2020 – 08/2020	Postdoctoral Research Associate Department of Chemistry, University of Cambridge, Cambridge, UK Supervisor: Prof. David Wales
08/2018 – 10/2018	Research Internship Q-Chem Inc., 6601 Owens Drive, Pleasanton, CA, USA

EDUCATION

10/2016 - 04/2020	PhD in Chemistry , Department of Chemistry, University of Cambridge, UK Title: Holomorphic Hartree–Fock Theory: Moving Beyond the Coulson–Fischer Point Supervisor: Dr Alex Thom
10/2012 - 06/2016	MA and MSci, Natural Sciences , Robinson College, University of Cambridge, UK <i>4th Year:</i> 1st Class (3 rd out of 58) <i>3rd Year:</i> 1st Class (3 rd out of 91) <i>2nd Year:</i> 1st Class (5 th out of 564) <i>1st Year:</i> 1st Class (9 th out of 614)

AWARDS, FELLOWSHIPS, AND FUNDING

2020–Present	Astor Junior Research Fellow in Chemistry , New College, Oxford Awarded a highly competitive, three-year stipendiary fellowship to independently develop my research.
2020	Outstanding Thesis Award , Department of Chemistry, University of Cambridge Awarded for the most outstanding PhD thesis in theoretical chemistry. Included a £500 prize.
2016–2020	Vice-Chancellor's Award , Cambridge Trust, University of Cambridge Fully-funded three-year PhD scholarship awarded in recognition of an outstanding undergraduate performance as one of the highest-scoring applicants.
Summer 2015	Undergraduate Research Bursary , Royal Society of Chemistry Funding for a summer research project, awarded to students with the greatest research potential.
2013–2020	Robinson College, University of Cambridge <ul style="list-style-type: none">• Elected into College Senior Scholarship (2016–2020)• Lewis Prize in Chemistry (2016)• Warden's Prize (2014)• College Prize for Natural Sciences (2014)• College Prize (2013, 2014, 2015 and 2016)• Elected into College Scholarship (2013–2016)
2013–16	Department of Chemistry, University of Cambridge <ul style="list-style-type: none">• Best first-year PhD peer-to-peer presentation (2016)• Gordon Wigan Prize for an outstanding performance in Part III Chemistry (2016)• BP Prize for an outstanding performance in Part II Chemistry (2015)• BP Prize for an outstanding performance in Part IB Chemistry B (2014)• BP Prize for an outstanding performance in Part IB Chemistry A (2014)

PUBLICATIONS

- [17] Yi Sun, and **H. G. A. Burton** (Submitted to *J. Chem. Phys.*)
Complex Analysis of Divergent Perturbation Theory at Finite Temperatures
- [16] **H. G. A. Burton**, *J. Chem. Theory Comput.* **18**, 1512 (2022)
Energy Landscape of State-Specific Electronic Structure Theory
- [15] E. Epifanovsky et. al, *J. Chem. Phys.* **155**, 084801 (2021)
Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package
- [14] **H. G. A. Burton**, C. Marut, T. J. Daas, P. Gori-Giorgi, and P.-F. Loos, *J. Chem. Phys.* **155**, 054107 (2021)
Variations of the Hartree–Fock Fractional-Spin Error for One Electron
- [13] **H. G. A. Burton**, *J. Chem. Phys.* **154**, 144109 (2021)
Generalised Nonorthogonal Matrix Elements: Unifying Wick’s Theorem and the Slater–Condon Rules
- [12] **H. G. A. Burton**, *J. Chem. Phys.* **154**, 111103 (2021)
Hartree–Fock Critical Nuclear Charge in Two-Electron Atoms [2021 Emerging Investigators Special Collection]
- [11] A. Marie, **H. G. A. Burton**, and P.-F. Loos, *J. Phys. Condens. Matter* **33**, 283001 (2021)
Perturbation Theory in the Complex Plane: Exceptional Points and Where to Find Them
- [10] **H. G. A. Burton** and D. J. Wales, *J. Chem. Theory Comput.* **17**, 151 (2021)
Energy Landscapes for Electronic Structure
- [9] R. A. Zarotiadis, **H. G. A. Burton** and A. J. W. Thom, *J. Chem. Theory Comput.* **16**, 7400 (2020)
Towards a Holomorphic Density-Functional Theory
- [8] **H. G. A. Burton** and A. J. W. Thom, *J. Chem. Theory Comput.* **16**, 5586 (2020)
Reaching Full Correlation through Nonorthogonal Configuration Interaction: A Second-Order Perturbative Approach
- [7] **H. G. A. Burton** and A. J. W. Thom, *J. Chem. Theory Comput.* **15**, 4851 (2019)
General Approach for Multireference Ground and Excited States using Nonorthogonal Configuration Interaction
- [6] **H. G. A. Burton**, A. J. W. Thom and P.-F. Loos, *J. Chem. Theory Comput.* **15**, 4374 (2019)
Parity-Time Symmetry in Hartree–Fock Theory [Selected for cover illustration]
- [5] S. Cardamone, J. R. R. Kimmitt, **H. G. A. Burton**, T. J. Todman, S. Li, W. Luk and A. J. W. Thom, *Int. J. Quantum Chem.* **119**, e25853 (2019)
Field-programmable gate arrays and quantum Monte Carlo: Power efficient coprocessing for scalable high-performance computing
- [4] **H. G. A. Burton**, A. J. W. Thom and P.-F. Loos, *J. Chem. Phys.* **150**, 041103 (2019)
Complex Adiabatic Connection: A Hidden Non-Hermitian Path from Ground to Excited States
- [3] **H. G. A. Burton**, M. Gross and A. J. W. Thom, *J. Chem. Theory Comput.* **14**, 607 (2018)
Holomorphic Hartree–Fock Theory: The Nature of Two-Electron Problems
- [2] Y. Liu, R. Ganti, **H. G. A. Burton**, X. Zhang, W. Wang, and D. Frenkel, *Phys. Rev. Lett.* **119**, 224502 (2017)
Microscopic Marangoni Flows Cannot Be Predicted on the Basis of Pressure Gradients
- [1] **H. G. A. Burton** and A. J. W. Thom, *J. Chem. Theory Comput.* **12**, 167 (2016)
Holomorphic Hartree–Fock Theory: An Inherently Multireference Approach

EXTERNAL PRESENTATIONS

Oral Presentations:

(* Invited speaker)

- [10] * March 2022 — CEFL-DESY Theory Seminar, University of Hamburg, Germany:
Energy Landscape of State-Specific Electronic Structure
- [9] September 2021 — 57th Symposium on Theoretical Chemistry (online):
Electronic Structure as an Energy Landscape: An Orbital-Free Perspective
- [8] * July 2021 — Computational Chemistry Seminar, University of Cardiff, UK:
Energy Landscape of Electronic Structure Theory
- [7] * June 2021 — Theoretical Physics Colloquium, Universität Duisburg–Essen, Germany:
Energy Landscape of Electronic Structure Theory
- [6] March 2021 — Faraday Joint Interest Group Conference, Sheffield, UK:
Efficient Potential Energy Surfaces using Multiple Hartree–Fock Solutions
- [5] * February 2021 — QuNB Seminar, University of New Brunswick, Canada:
Strong Correlation using Multiple Hartree–Fock Solutions
- [4] * October 2019 — LCPQ Seminar Series, Université Paul Sabatier, France:
Multireference Ground and Excited States using Multiple Hartree–Fock Solutions
- [3] * August 2018 — Head–Gordon Group Seminar, University of California, Berkeley, USA:
Holomorphic Hartree-Fock Theory: Exploiting Symmetry-Breaking in Non-Orthogonal CI
- [2] June 2018 — Satellite meeting to the 16th International Congress of Quantum Chemistry, Strasbourg, France:
Holomorphic Hartree-Fock Theory: Strong Correlation and the Existence of Multiple Hartree–Fock Solutions
- [1] * October 2017 — Theory Research Interest Group, Department of Chemistry, University of Cambridge, UK:
Holomorphic Hartree-Fock Theory: Exploiting Multiple SCF Solutions for Non-Orthogonal Configuration Interaction

Poster Presentations:

- [5] July 2019 — 10th Congress of the International Society for Theoretical Chemical Physics (Tromsø, Norway):
“Non-Hermitian Quantum Chemistry: Electronic Structure in the Complex Domain”
- [4] June 2019 — 9th Molecular Quantum Mechanics Conference (Heidelberg, Germany):
“Holomorphic Hartree–Fock Theory: A General Approach for Multireference Systems”
- [3] June 2018 — 16th International Congress of Quantum Chemistry (Menton, France):
“Holomorphic Hartree–Fock Theory: Restoration of Excited States using NOCI”
- [2] August 2017 — 11th Congress of the World Association of Theoretical and Computational Chemistry (Münich, Germany):
“Holomorphic Hartree–Fock Theory: Beyond the Coulson–Fischer Point”
- [1] March 2017 — Computational Molecular Science 2017 (Warwick, UK):
“Holomorphic Hartree–Fock Theory: Beyond the Coulson–Fischer Point”

MAJOR COLLABORATIONS

- Prof. David Tew — University of Oxford, UK
- Dr Pierre-François Loos — Université Paul Sabatier, Toulouse, France
- Prof. David Wales — University of Cambridge, UK
- Prof. Stijn De Baerdemacker — University of New Brunswick, Canada

OUTREACH, SERVICE, AND ENGAGEMENT

Outreach and Admissions:

- Interviewed for undergraduate chemistry admissions at St. Hilda's College, Oxford (2021)
- Student representative at the Robinson College admissions conference for teachers (2019)
- Chemistry demonstrator for the Cambridge Science Festival (2015)
- Student guide for the Robinson College undergraduate open days (2013–2015)

Academic Peer Review:

- Journal of Chemical Theory and Computation
- Journal of Physical Chemistry Letters
- Journal of Physics: Condensed Matter
- Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences
- Journal of Physics B: Atomic, Molecular and Optical Physics

Departmental Representation:

- Student representative on the Chemistry Consultative Committee at the University of Cambridge (2013–14)

Software Development:

- Developer for the commercial quantum-chemistry program Q-Chem, based in California, USA.
- Awarded a competitive internship at Q-Chem to develop my PhD research into a production code.

TEACHING EXPERIENCE

Supervision of Research Projects:

University of Oxford:

2021–22	Principal supervisor for an erasmus masters research project.
2021–22	Principal supervisor for an integrated masters research project.
Summer 2021	Principal supervisor for a 6-week undergraduate summer research project.

University of Cambridge:

2019–20	Day-to-day supervisor for a 16-week undergraduate research project.
2018–19	Day-to-day supervisor for an erasmus masters student.
2018–19	Day-to-day supervisor for a 16-week undergraduate research project.
Summer 2017	Day-to-day supervisor for an 8-week summer undergraduate research project.

Undergraduate Teaching:

University of Oxford:

2021–22	Tutor for second-year supplementary course on quantum chemistry.
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University of Cambridge:

2018–20	Supervisor for third-year theoretical chemistry course on symmetry.
2017–18	Laboratory demonstrator for third-year theoretical chemistry.
2016–17	Supervisor for second-year physical and theoretical chemistry course.
2016–19	Supervisor for first-year general chemistry course.
2016–17	Laboratory demonstrator for first-year general chemistry.