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 *4th Year:* **1st Class** (3rd out of 58) *3rd Year:* **1st Class** (3rd out of 91) *2nd Year:* **1st Class** (5th out of 564) *1st Year:* **1st Class** (9th out of 614)

Awards, Fellowships, and Funding

September 2022	**Researcher Development Grant**, Royal Society of Chemistry Awarded £500 to attend an international conference as an invited speaker.
July 2022	**Lockey Fund**, MPLS Division, University of Oxford Awarded £770 to attend a major international conference.
2020–Present	**Astor Junior Research Fellow in Chemistry**, New College, Oxford Awarded a highly competitive, three-year stipendiary fellowship to independently develop my research [equivalent to £75,000, including an annual research budget of £1,380].
2020	**Outstanding Thesis Award**, Department of Chemistry, University of Cambridge Awarded for the most outstanding PhD thesis in theoretical chemistry [£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 [equivalent to £42,000].
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** • 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** • 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)

Research Activities and Interests

- Development of electronic structure algorithms for quantum computing.
- Mathematical analysis of electronic wave function approximations.
- Multiple solutions and symmetry breaking in electronic structure methods.
- Nonorthogonal computational methods for strong electron correlation.
- Non-Hermitian quantum mechanics and complex analysis of perturbation theories.

PUBLICATIONS

[22] A. Marie, and **H. G. A. Burton**, *Submitted* (2023)
Excited states, symmetry breaking, and unphysical solutions in state-specific CASSCF theory

[21] D.-G. Oprea, and **H. G. A. Burton**, *In Press* (2023)
Convergence of Møller–Plesset perturbation theory for excited reference states

[20] S. De Baerdemacker, A. Ayati, **H. G. A. Burton**, X. De Vriendt, P. Bultinck, and G. Acke, *Submitted* (2023)
Spin-constrained Hartree–Fock and the generator coordinate method for the 2-site Hubbard model

[19] **H. G. A. Burton**, D. Marti-Dafcik, D. P. Tew, and D. J. Wales, *Submitted* (2022)
Exact electronic states with shallow quantum circuits through global optimisation

[18] **H. G. A. Burton**, *J. Chem. Phys.* **157**, 204109 (2022)
Generalized nonorthogonal matrix elements. II: Extension to arbitrary excitations

[17] Y. Sun, and **H. G. A. Burton**, *J. Chem. Phys.* **156**, 171101 (2022)
Complex analysis of divergent perturbation theory at finite temperature

[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)

[16] * November 2022 — Chemical Institute of Canada: PTC-Virtual Seminar (online):
Globally Optimised Unitary Product States for Exact Electronic Structure

[15] * October 2022 — Warwick Computational Chemistry Seminar, Warwick, UK:
Modernising Electronic Structure Theory for Challenging Ground and Excited States

[14] September 2022 — RSC Theoretical Chemistry Group Early Career Meeting (online):
Globally Optimised Unitary Product States for Exact Electronic Structure

[13] * September 2022 — 6th International Conference on Molecular Electronic Structure, Monastir, Tunisia:
Multiple Solutions in Electronic Structure: Excited States, Symmetry Breaking, and Strong Correlation

[12] * July 2022 — SciCADE 2022, Reykjavik, Iceland:
Energy Landscape of Electronic Structure Theory

[11] July 2022 — 11th Congress of the World Association of Theoretical and Computational Chemistry, Vancouver, Canada:
Universal Fermionic Simulations using Minimal Operators

[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] * Feburary 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
- Prof. David Wales — University of Cambridge, UK
- Dr Pierre-François Loos — Université Paul Sabatier, Toulouse, France
- Prof. Stijn De Baerdemacker — University of New Brunswick, Canada
- Dr George Booth — King's College London, UK

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.

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.