Hugh G. A. Burton

Employment

10/2020 – Present	**Astor Junior Research Fellow in Chemistry** New College, Oxford, UK **Academic Visitor** 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

2020–Present	**Astor Junior Research Fellow in Chemistry**, New College, Oxford Awarded a highly competitive, stipendiary Research Fellowship for three years to independently develop my research proposal.
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 an 8-week 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)

Publications

[14] **H. G. A. Burton**, C. Marut, T. J. Daas, P. Gori-Giorgi, and P.-F. Loos *Submitted to J. Chem. Phys.* (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)

[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 Triennial 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

- 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
- Prof. Eric Neuscamman — University of California, Berkeley, USA

Outreach, Service, and Engagement

Quantum Chemistry Software Development:

- Software 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 for the wider academic and industrial science community, now available on the latest global release.

Academic Peer Review:

- Journal of Physical Chemistry Letters
- Journal of Chemical Theory and Computation

Departmental Representation:

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

Outreach and Admissions:

- 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)

Teaching Experience

Supervision of Research Projects:

2021–22	Principal supervisor for an upcoming Erasmus Masters student.
2021–22	Principal supervisor for an upcoming integrated masters research project.
Summer 2021	Principal supervisor for a 6-week summer undergraduate research project.
2019–20	Day-to-day supervisor for a 16-week undergraduate research project.
2018–19	Day-to-day supervisor for an Erasmus Masters student, resulting in a publication.
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:

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.