Hugh G. A. Burton

Employment

10/2020–Present	**Kim and Julianna Silverman Research Fellow** Downing College, Cambridge, UK **Visiting Researcher** Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, UK
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 Theoretical 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

July 2023	**Kim and Julianna Silverman Research Fellow**, Downing College, Cambridge Prestigious 3-year research fellowship to pursue independent research. [Approx. £100,000].
November 2022	**Access to High Performance Computing**, EPSRC Co-investigator on a 1-year project to benchmark new quantum computational chemistry algorithms. [Equivalent to £10,074].
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 as a speaker.
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 Scholarship (2013–2016) and Senior Scholarship (2016–2020) • Lewis Prize in Chemistry (2016) • Warden's Prize and College Prize for Natural Sciences (2014) • College Prize for 1st Class examination results (2013, 2014, 2015 and 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

- Mathematical analysis of higher-energy solutions in electronic wave function approximations.
- Development of electronic structure algorithms for quantum computing.
- Nonorthogonal computational methods for strong electron correlation.
- Non-Hermitian quantum mechanics and the complex analysis of perturbation theory.

Professional Skills and Abilities

Leadership and Pastoral Care

- Instigated and led a multi-centre collaboration with David Tew (University of Oxford), and David Wales (University of Cambridge).
- Principal supervisor for two fourth-year masters students, including designing their research projects.
- Pastoral advisor for graduate students at New College, Oxford.

Management of Research Time, Data, and Grant Funding

- Attended professional development courses on Project Management, organised by the University of Oxford Career's Service.
- Budgeted my fellowship research allowance alongside external funding to attend multiple major international conferences.
- Maintain my own version-controlled research software and provide open-source data with all publications.
- Experience in balancing diverse commitments including undergraduate teaching, project supervision, multiple ongoing research collaborations, preparing publications, applying for funding, and peer reviewing for journals.

Communication and International Reputation

- Developed an extensive personal network of contacts, resulting in invited seminars at universities around the world.
- Invited to give oral presentations at major international conferences.
- Publications in the *Emerging Investigators Special Collections* of the Journal of Chemical Physics.
- Invited submission for the *Early-Career & Emerging Researchers in Physical Chemistry* edition of the Journal of Physical Chemistry.
- Maintain a professional website and Twitter account with over 1000 followers.

Collaboration and Interdisciplinary Research

- Established an interdisciplinary collaboration with mathematician Mark Gross (University of Cambridge), resulting in a publication.
- Ongoing national and international collaborations that have lead to several publications and academic research visits.
- Software developer for the commercial quantum chemistry program Q-Chem, based in California, USA. Awarded a competitive internship to develop my PhD research into a production code.

Outreach, Service, and Engagement

Professional Associations:

- Member of the Royal Society of Chemistry

Outreach and Admissions:

- Interviewed for undergraduate chemistry admissions at St. Hilda's College, Oxford (2021, 2022)
- 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:

- *2022 Outstanding Reviewer Award* for the Journal of Physics B: Atomic, Molecular and Optical Physics
- Awarded *Trusted Reviewer Status* by the Institute of Physics
- 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

Administrative Duties:

- Attend fortnightly departmental administration meetings in the Physical and Theoretical Chemistry Laboratory (Oxford).
- Student representative on the Chemistry Consultative Committee at the University of Cambridge (2013–14).
- Six years of committee experience for Robinson College Boat Club (2013–2019), including a year as President.

Major Collaborations

- Prof. David Tew — University of Oxford, UK
- Prof. David Wales — University of Cambridge, UK
- Dr Pierre-François Loos — Université de Toulouse, France
- Prof. Stijn De Baerdemacker — University of New Brunswick, Canada
- Dr George Booth — King's College London, UK

External Presentations

Oral Presentations:

(* Invited speaker)

20. * September 2023 — Theory and Molecular Simulation in the Physical Sciences, Cambridge, UK:
    Systematically improvable electronic wave functions for quantum computing
19. * June 2023 — 17th International Congress of Quantum Chemistry, Bratislava, Slovakia:
    Excited states, symmetry breaking, and multiple solutions in electronic structure theory
18. * June 2023 — Satellite meeting to the 17th International Congress of Quantum Chemistry, Znojmo, Czechia:
    Unitary product states: A quantum-compatible approach for strong correlation
17. * March 2023 — Lennard-Jones Centre Discussion Group, University of Cambridge, UK:
    Excited states, symmetry breaking, and multiple solutions in electronic structure theory
16. * February 2023 — TSCM Seminar, King's College London, UK:
    How to build a wave function with a quantum circuit: Globally optimised unitary product states for exact electronic structure
15. * November 2022 — Chemical Institute of Canada: PTC-Virtual Seminar (online):
    Globally Optimised Unitary Product States for Exact Electronic Structure
14. * October 2022 — Warwick Computational Chemistry Seminar, University of Warwick, UK:
    Modernising Electronic Structure Theory for Challenging Ground and Excited States
13. September 2022 — RSC Theoretical Chemistry Group Early Career Meeting (online):
    Globally Optimised Unitary Product States for Exact Electronic Structure
12. * September 2022 — 6th International Conference on Molecular Electronic Structure, Monastir, Tunisia:
    Multiple Solutions in Electronic Structure: Excited States, Symmetry Breaking, and Strong Correlation
11. * July 2022 — SciCADE 2022, Reykjavik, Iceland:
    Energy Landscape of Electronic Structure Theory
10. July 2022 — 11th Congress of the World Association of Theoretical and Computational Chemistry, Vancouver, Canada:
    Universal Fermionic Simulations using Minimal Operators
9. * March 2022 — CEFL-DESY Theory Seminar, University of Hamburg, Germany:
    Energy Landscape of State-Specific Electronic Structure
8. September 2021 — 57th Symposium on Theoretical Chemistry (online):
    Electronic Structure as an Energy Landscape: An Orbital-Free Perspective
7. * July 2021 — Computational Chemistry Seminar, University of Cardiff, UK:
    Energy Landscape of Electronic Structure Theory
6. * June 2021 — Theoretical Physics Colloquium, Universität Duisburg–Essen, Germany:
    Energy Landscape of Electronic Structure Theory
5. March 2021 — Faraday Joint Interest Group Conference, Sheffield, UK:
    Efficient Potential Energy Surfaces using Multiple Hartree–Fock Solutions
4. * February 2021 — QuNB Seminar, University of New Brunswick, Canada:
    Strong Correlation using Multiple Hartree–Fock Solutions
3. * October 2019 — LCPQ Seminar Series, Université Paul Sabatier, France:
    Multireference Ground and Excited States using Multiple Hartree–Fock Solutions
2. * August 2018 — Head–Gordon Group Seminar, University of California, Berkeley, USA:
    Holomorphic Hartree-Fock Theory: Exploiting Symmetry-Breaking in Non-Orthogonal CI
1. 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

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"

List of Publications

22. **H. G. A. Burton**, D. Marti-Dafcik, D. P. Tew, and D. J. Wales, *npj Quantum Inf.* **9**, 75 (2023)
    Exact electronic states with shallow quantum circuits through global optimisation
21. A. Marie, and **H. G. A. Burton**, *J. Phys. Chem. A* **127**, 4538 (2023)
    Excited states, symmetry breaking, and unphysical solutions in state-specific CASSCF theory [Cover article]

20. S. De Baerdemacker, A. Ayati, **H. G. A. Burton**, X. De Vriendt, P. Bultinck, and G. Acke, *Adv. Quantum Chem.* **88**, 161 (2023)
Spin-constrained Hartree–Fock and the generator coordinate method for the 2-site Hubbard model
19. D.-G. Oprea, and **H. G. A. Burton**, *Adv. Quantum Chem.* **88**, 249 (2023)
Convergence of Møller–Plesset perturbation theory for excited reference states
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 [2022 Emerging Investigators Special Collection]
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

Teaching Experience

Supervision of Research Projects:

University of Oxford:

2022–23	Principal supervisor for an integrated masters research project.
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:

2021–23	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.
2016–19	Supervisor for first-year general chemistry course.
2016–17	Supervisor for second-year physical and theoretical chemistry course.
2016–17	Laboratory demonstrator for first-year general chemistry.