

# Hugh G. A. Burton

## EMPLOYMENT

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

## EDUCATION

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

## AWARDS, FELLOWSHIPS, AND FUNDING

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

## PUBLICATIONS

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- [16] H. G. A. Burton (Submitted to *J. Chem. Theory Comput.*)  
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

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### Oral Presentations:

#### (\* Invited speaker)

- [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

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

## OUTREACH, SERVICE, AND ENGAGEMENT

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### 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

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

## TEACHING EXPERIENCE

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### 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.