Biographical Sketch

James Daniel Whitfield

Contact

Dartmouth College, Department of Physics & Astronomy
6127 Wilder Laboratory, Room 248
Hanover, New Hampshire 03755-3528

(603) 646-1110
James.D.Whitfield@dartmouth.edu
jdwhitfield.com

Education

2011-2006	**Ph.D. Chemical Physics**, Harvard University Thesis: *At the Intersection of Quantum Computing and Quantum Chemistry* Advisor: Alán Aspuru-Guzik
2009-2006	**A.M. Chemistry**, Harvard University
2006-2003	**B.S. Mathematics and Chemistry**, *Magna cum laude*, Morehouse College

Academic Appointments

2022-Present	**Associate Professor of Physics**, Dartmouth College Department of Physics and Astronomy
2016-2022	**Assistant Professor of Physics**, Dartmouth College Department of Physics and Astronomy
2020-Present	**Adjunct Assistant Professor of Chemistry**, Dartmouth College Department of Chemistry

Non Academic Appointments

2021-Present	**Amazon Visiting Academic**, Amazon Web Services
2019-2021	**Chief Scientific Advisor**, qBraid.com

Consulting Experience

2024-Present	**Advanced Scientific Computing Advisory Committee** member, Department of Energy
2020-Present	**Research Advisory Board**, IBM Historically Black Colleges and Universities Quantum Center
2020-Present	**Scientific Advisory Board**, *Qubit by Qubit* at The Coding School
2020-2021	**Chief Scientific Advisor**, qBraid.com
2020-2021	**Scientific Advising Board**, Zapata Computing

Funding, Fellowships, and Awards Since 2016

2024-2027 "Optimal Basis Set Design for Computational Chemistry Basis Set Design," PI
Army Research Office: $390k

2019-2023 "Harnessing the Data Revolution for the Quantum Leap," Co-I
National Science Foundation: $1,949k

2019-2024 "Fundamental Algorithmic Research for Quantum Computing (FAR-QC)," Co-PI
Department of Energy: $750k

2021-2024 "Quantum Chemistry for Quantum Computers (QCQC)," Co-PI
Department of Energy: $407k

2019-2024 "Optimization, Verification, and Engineered Reliability of Quantum Computers (OVER-QC)," Co-PI
Department of Energy: $727k

2018-2022 "Topological Fermionic Quantum Simulation (PHYS-1820747)," PI
National Science Foundation: $385k

Postdoctoral Fellowships

2015-2016 **Postdoctoral Fellow**, University of Ghent (Ghent, Belgium)
Advisor: Frank Verstraete

2012-2015 **VCQ Postdoctoral Fellow**, Vienna Center for Quantum Science and Technology (Vienna, Austria)
Advisor: Frank Verstraete

2011-2012 **Postdoctoral Fellow**, Columbia University (New York, NY)
Advisor: Boris Altshuler

2011-2012 **Postdoctoral Fellow**, NEC Laboratories America (Princeton, NJ)
Advisor: Jérémie Roland

Awards

2014-2015 Ford Postdoctoral Fellowship, Ford Foundation

2011 Molecular Physics Young Author Prize for paper: "Simulation of Electronic Structure Hamiltonians using Quantum Computers," *Molecular Physics* 109(5): 735-750, 2011.

2006-2011 Harvard University Graduate Prize Fellowship, Harvard University

Teaching

2016-2021 Physics 73: *Introduction to Condensed Matter*
Fall 2020, Fall 2018, Fall 2017, Fall 2016

2017-2021 Physics 40: *Quantum Physics of Matter*
Spring 2021, Spring 2019, Spring 2017

2022 Physics 113: *Microscopic Theory of Solids*
Winter 2022

2018-2021 Physics 13: *Introductory Mechanics*
Winter 2021, Winter 2020, Winter 2019, Winter 2018

2018-2022 Physics 116: *Quantum Information Science*
Spring 2024, Spring 2022, Spring 2020, Spring 2018

2024 Physics 44: *Classical Mechanics*
Summer 2024

Undergraduate Theses Supervised as Primary Advisor

2021 Omar Alsaeed — Department of Physics at Middlebury College
Simulating Hamiltonian Dynamics Using Product Formulas (co-supervised with Chris Herdman)

2019 Shaket Chaudhary — Department of Computer Science Honors Thesis
Constructing Random Ensembles of Fermionic Systems (co-supervised with Prof. Bo Zhu)

2018 Erik Weis — Department of Physics and Astronomy Honors Thesis
Benchmarking Quantum Computers Using Electronic Structure Algorithms

2017 Samuel Greydanus — Department of Physics and Astronomy Honors Thesis
Approximating Matrix Product States with Machine Learning

Post-baccalaureate Supervision

Summer 2020	Phyo Pyi Kyaw	Benchmarking Ground State Energy Computations Using PySCF and ACCDB
Summer 2019	Kent Ueno	Quantum computer interfaces
2017-2018	Tarini Hardikar	Quantum chemistry on quantum computers
Summer 2016	Vojtech Havlíček	Spin-to-fermion transforms

PhD Theses Supervised

2023 Riley Chien — Department of Physics and Astronomy PhD Thesis
Fermion Encodings and Algorithms For Quantum Simulation

2023 Jun Yang — Department of Physics and Astronomy PhD Thesis
Machine Learning For Electronic and Atomistic Simulations

2020 Kanav Setia — Department of Physics and Astronomy PhD Thesis
Fermionic Quantum Simulation

Women In Science Project Interns Supervised

Spring 2021	Hadiye Nisa Kuvvett (c/o 2024)
	Emily Schuster (c/o 2024)
Fall 2019	Katherine F. Lasonde (c/o 2023)
	Alana Macken (c/o 2023)
Fall 2018	Junqing (Ivy) Yan (c/o 2022)
Fall 2017	Aiko D. Takata (c/o 2021)
	Margaret L. Hubble (c/o 2021)

Service to the Profession

2024 Organizing committee member for Quantum Noir 2024 hosted at Harvard University
2024 Long-term visitor at Simons Institute for the Theory of Computing Workshop *The Quantum Wave in Computing*. UC Berkeley
2023 Panelist and reviewer for Ford Foundation Fellowship Programs. Ford Foundation
2020 Organizer of Quantum Winter School [Virtual]. Dartmouth College
2020 Panelist at the Kickoff National Q-12 Education Partnership [Virtual]. White House
2020 Long-term visitor at Simons Institute for the Theory of Computing Workshop *The Quantum Wave in Computing*. UC Berkeley
2020 Participant (qBraid.com) as part of *MIT Delta V 2020 accelerator* summer 2020 cohort [Virtual]. MIT
2020 Organizer and facilitator for two-week Quantum Computing Introduction using qBraid.com. Hanover High School
2019 Participant at Achieving a Quantum Smart Workforce Workshop. Kavli Futures Symposium
2018 Participant at Summit on Advancing American Leadership in Quantum Information Science. White House
2018 Long-term visitor at Simons Institute for the Theory of Computing Workshop *Challenges in Quantum Computing*. UC Berkeley
2018 Participant at National Science Foundation Young Investigator's Workshop. NSF Headquarters
2017 Participant at The Physics and Astronomy New Faculty Workshop. American Association of Physics Teachers
2017 Panelist and reviewer for Ford Foundation Fellowship Programs. Ford Foundation
2015 Co-organizer for *Novel Computing Approaches to Quantum Chemistry* conference, Telluride Science Research Center
2012 Long-term visiting scholar at Condensed Matter Group. Max Planck Institute for the Physics of Complex Systems
2012 Visiting scientist at Quantum Science Laboratory. Institute for Scientific Interchange

Reviewer for various journals (*Quantum Information and Computation*, *New Journal of Physics*, *Nature*, *Nature Physics*, *Nature Communications*, *Physical Review A*, *Physical Review Letters*, *Quantum Science and Technology*, *Journal of Physics A: Mathematical and Theoretical*, *International Journal of Quantum Chemistry*, National Science Foundation Ad-Hoc panels, *Alexander von Humboldt Fellowship* reviewer, *Mitacs Foundation* proposal reviewer)

Department Committees

2021-2022 Faculty Search Committee Member
2021-2022 Science Department Climate Survey Response Team, Department of Physics and Astronomy Representative
2016-2022 Department Webpage and Digital Outreach Committee Chair
2018-2019 Department Colloquium Committee Member
2016-2019 Graduate Admissions and Policy Committee Member

College Committees

2024 - present Dartmouth College Committee on Standards
2018-2019 Faculty Search Committee, William H. Neukom Academic Cluster in Computational Science

Talks since 2016

Conference and Workshop Presentations

1. The SIAM Quantum Intersections Convening (invited speaker) — Tysons, VA — October 2024
    - Overview of Quantum Chemistry — October 8, 2024
2. Quantum Noir Workshop (invited speaker) — Harvard University — June 2024
    - Delivering Quantum Technology: An Amazon Visiting Academic perspective — June 11, 2024
    - Mentoring Panel (panelist) — June 15, 2024
3. CERAWeek 2023 — S&P Global — Houston, TX — February 2023
    - Industry panel: The Continued Expansion of Quantum Technology in the Energy Ecosystem (panelist) — March 9, 2023
4. HSI-SIS Quantum Information Sciences Summit — University of California, Davis [Virtual] — April 2022
    - QIS Pedagogy Plenary Panel — April 26, 2022
5. BRICvt X qBraid: Quantum Computing Summit (invited speaker) — Black River Innovation Campus [Virtual] — September 2021
    - How to Understand Quantum Mechanics: The Probability-First Approach — September 24, 2021
6. Useful Quantum Computation For Quantum Chemistry (keynote speaker) — Lorentz Center (Leiden, Netherlands) [Virtual] — February 2021
    - Hybrid quantum computing: quantum-classical interfaces — February 22, 2021
7. QIS Education Workshop: Effecting Systemic Change in QIS Education — National Q-12 Education Partnership [Virtual] — February 2021
    - QIS Education at the K-12 level (invited panelist) — February 24, 2021
8. Quantum Winter School 2020 (invited lecturer) — Dartmouth College [Virtual] — December 2020
    - Welcome to the Quantum World — December 14, 2020
    - Quantum Computing for Chemistry and Materials — December 16, 2020
9. Q-Turn 2020: Changing paradigms in quantum science (invited speaker) — [Virtual] — November 2020
    - Simulating fermions with qubits — November 24, 2020
10. Theoretical Physics Symposium 2019 (invited speaker) — DESY Hamburg, Germany — November 2019
    - Quantum technology and time-dependent density functional theory — November 15, 2019
11. Quantum Information for Developers Summer School and Hackathon (invited lecturer) — Swiss Federal Institute of Technology in Zürich, Switzerland — September 2019
    - Hamiltonian Simulation Problems and Quantum Chemistry — September 8, 2019
    - Fermions, bosons, and qubits — September 8, 2019
    - Time evolution and measurements of Hamiltonians — September 9, 2019
12. Quantum Indeterminacy Workshop (invited speaker) — Dartmouth College — July 2019
    - Computation versus Experiment: Quantum Technology Meets Quantum Computing — July 13, 2019

13. American Physical Society Meeting (speaker) — Boston, MA — March 2019

    - Quantum Simulation and Time-Dependent Density Functional Theory. Session: Applications of Noisy Intermediate Scale Quantum Computers III. — March 5, 2019

14. Mathematics Society Joint Mathematics Meeting (speaker) — Baltimore, MD — January 2019

    - Quantum Measurement Problem. Session: AMS Special Session on 25 years of Conferences for African-American Researchers in the Mathematical Sciences (CAARMS times 25), II — January 16, 2019

15. International Workshop on Quantum Chemical Calculations on Quantum Computers (invited speaker) — Osaka City University, Japan — March 2018

    - Fermionic Algebras for Quantum Computing — March 29, 2018

Invited Seminars/Colloquiums

1. University of Texas at Dallas — Perfect Matchings, Planar Graphs, and Fermionic Systems — Quantum Information Science - Condensed Matter Physics Seminar — November 15, 2024

2. Argonne National Laboratory — Indistinguishability of fermions and quantum simulation — Argonne Physics Division Colloquium — June 7, 2024

3. Middlebury College — Quantum Theory: From Mechanics to Engineering — Computer Science Department Seminar — March 13, 2024.

4. University of California Berkeley — The Complexity of Fermions in Quantum Information and Beyond — Richard M. Karp Distinguished Lecture — March 11, 2024.

5. Massachusetts Institute of Technology — MIT Quantum Information Science and Engineering (iQuISE) Seminar — [virtual] — An Introduction to Fermions in QIS. October 5, 2023.

6. Harvard University — Quantum Information Seminar Series — Cambridge, MA — At The Intersection of Quantum Computing and Quantum Chemistry. September 14, 2023.

7. University of Iowa — Physics Department Seminar — [virtual] — Quantum Computing and Quantum Chemistry. March 3, 2023.

8. Tufts University — Physics and Astronomy Colloquium — Medford, MA — Basis Sets, Electronic Structure, and Quantum Computing. December 9, 2022.

9. DOE — AIDE — Free-Fermion Optimization. August 31, 2022 [virtual].

10. University of Washington — Quantum Information Science and Engineering Graduate Seminars — Seattle, WA — Rooftop Views of Quantum Algorithms. February 22, 2022 [Virtual].

11. Princeton University — Princeton Quantum Colloquium — Princeton, NJ — Individual Qubits and Indistinguishable Fermions. November 29, 2021.

12. Rice University — Quantum Seminar Series — Houston, TX — Indistinguishability and Computational Complexity of Fermions. September 8, 2021 [Virtual].

13. DOE Accelerated Research in Quantum Computing Seminar Series — Fermion Encodings and the Simulation of Quantum Chemistry. September 1, 2021 [Virtual].

14. The Coding School — Qubit by Qubit — Guest Spotlight. March 21, 2021 [Virtual].

15. University of South Florida — Department of Physics — Tampa Bay, FL — Quantum Computing for the Simulation of Electrons. March 19, 2021 [Virtual].

16. Dartmouth College — Women In Science Project Science Faculty Spotlight — Hanover, NH — January 28, 2021 [Virtual].

17. Pacific Northwest National Laboratories — Northwest Quantum Nexus Seminar — Seattle, WA — Hartree-Fock and Quantum Technology. January 20, 2021 [Virtual].

18. Williams College — Department of Physics — Williamstown, MA — Welcome to Quantum: Moving from Mechanics to Engineers. October 30, 2020 [Virtual].

19. Dartmouth College — Department of Mathematics — Hanover, NH — An Invitation to Quantum: Concepts, Technology, and Dartmouth. October 20, 2020 [Virtual].

20. University of Illinois Urbana-Champaign — Institute for Condensed Matter Theory Seminar — Urbana, IL — Quantum Simulation of Fermions. October 12, 2020 [Virtual].

21. University of Maryland, College Park — Joint Quantum Institute — College Park, MD — Limitations of Hartree-Fock Using Quantum Resources. September 23, 2020 [Virtual].

22. Dartmouth College — Department of Physics and Astronomy — Hanover, NH — Quantum Technology: Here and Now. April 15, 2020 [Virtual].

23. Harvard University — Institute for Theoretical Atomic Molecular and Optical Physics — Cambridge, MA — Quantum Computing and Non-interacting Electronic Theories. November 7, 2019.

24. Naval Research Laboratory — Chemistry Colloquium — Washington, D.C. — Chemistry in the Age of Quantum Supremacy. October 17, 2019.

25. Stony Brook University — Stony Brook, NY — Quantum Simulation of Fermions: Fermion-to-Spin Mappings and TDDFT. May 16, 2019.

26. Bates College — Physics and Astronomy — Lewiston, ME — The Promise of Quantum Technology. November 15, 2018.

27. Virginia Institute of Technology — Department of Physics — Blacksburg, VA — Quantum Simulation of Fermions. September 10, 2018.

28. Microsoft — Azure Quantum Service — Redmond, WA — Quantum Simulation and Applications. August 9, 2018.

29. Pacific Northwest National Laboratories — Richland, WA — Quantum Simulation of Fermions. August 7, 2018.

30. Rigetti Quantum Computing — Berkeley, CA — Hydrogen Quantum Simulation. July 18, 2018.

31. Simons Institute for the Theory of Computing — Berkeley, CA — Formalizing Electronic Structure Problems. July 12, 2018.

32. Sandia National Laboratories — Livermore, CA — Quantum Simulation of Fermions. July 9, 2018.

33. IBM T. J. Watson Research Center — Yorktown Heights, NY — Fermionic Simulation on Quantum Computers. June 9, 2018.

34. Dartmouth College — E.E. Just Program Science Forum — Hanover, NH — Quantum Reflections. January 11, 2017.

35. Los Alamos National Laboratory — Quantum Lunch Seminar — Los Alamos, NM — Fermionic Algebras for Qubits. January 26, 2017 .

36. Georgia Institute of Technology — Quantum Information Seminar — Atlanta, GA — Electronic Structure on Quantum Computers with Ultra-Local Qubit Operators. January 31, 2017.

Scholarly Works

Citation metrics as reported by Google Scholar (h-index: 24, i10-index: 32)

1. A Projansky, J Neicase, J D Whitfield. Extending Simulability of Cliffords and Matchgates. (Preprint) arXiv:2410.10068, 2024.

2. T Henderson, B Harrison, I Magoulas, J Necaise, A Projansky, F Evangelista, J D Whitfield. Fermion Mean-Field Theory as a Tool for Studying Spin Hamiltonians. *Journal of Chemical Physics*, 161: 234112, 2024.

3. B Harrison, M Chiew, J Necaise, A Projansky, S Strelchuk, J D Whitfield. A Sierpinski Triangle Fermion-to-Qubit Transform (Preprint) arXiv:2409.04348, 2024.

4. R Dutta, D GA Cabral, N Lyu, N P Vu, Y Wang, B Allen, X Dan, R G Cortiñas, P Khazaei, S E Smart, S Nie, M H Devoret, D A Mazziotti, P Narang, C Wang, J D Whitfield, A K Wilson, H P Hendrickson, D A Lidar, F Pérez-Bernal, L F Santos, S Kais, E Geva, V S Batista. Simulating Chemistry on Bosonic Quantum Devices. *Journal of Chemical Theory and Computation*, 20 (15):64266441, 2024.

5. B Harrison, J Necaise, A Projansky, J D Whitfield. A Sierpinski Triangle Data Structure for Efficient Array Value Update and Prefix Sum Calculation. (preprint) arXiv:2403.03990, 2024.

6. A Projansky, J T Heath, J D Whitfield. Entanglement Spectrum of Matchgate Circuits with Universal and Non-Universal Resources. *Quantum*, 8:1432, 2024.

7. R W Chien, K Setia, X Bonet-Monroig, M Steudtner, J D Whitfield. Simulating Quantum Error Mitigation in Fermionic Encodings. (preprint) arXiv:2303.02270, 2023.

8. A Cupo, J T Heath, E Cobanera, J D Whitfield, C Ramanathan, L Viola. Optical Conductivity Signatures of Floquet Electronic Phases. *Physical Review B*, 108: 024308, 2023.

9. W Wang, J D Whitfield. Basis Set Generation and Optimization in the NISQ Era with Quiqbox.jl. *Journal of Chemical Theory and Computation*, 19 (22): 80328052, 2023.

10. J Yung, J D Whitfield. Machine-Learning Kohn-Sham Potential From Dynamics in Time-Dependent Kohn-Sham Systems. Machine Learning: Science and Technology, 4: 035022, 2023.

11. B OGorman, S Irani, J D Whitfield, and B Fefferman. Intractability of Electronic Structure in a Fixed Basis. *PRX Quantum*, 3: 020322, 2022.

12. B Harrison, D Nelson D Adamiak, J D Whitfield. Reducing the Qubit Requirement of Jordan-Wigner Encodings of N-mode, K-Fermion Systems from N to $\lceil \log_2 \binom{N}{K} \rceil$. (Preprint) arXiv:2211.04501, 2022.

13. J D Whitfield, J Yang, W Wang, J T Heath, B Harrison. Quantum Computing 2022 (Preprint) arXiv:2201.09877, 2022.

14. A Cupo, E Cobanera, J D Whitfield, C Ramanathan, L Viola. Floquet Graphene Antidot Lattices *Physical Review B*, 104: 174304, 2021.

15. S Gulania, J D Whitfield. Limitations of Hartree-Fock with Quantum Resources. *Journal of Chemical Physics*, 154: 044112, 2021.

16. J Yang, J Brown, J D Whitfield. A Comparison of Three Ways to Measure Time-Dependent Densities With Quantum Simulators. *Frontiers in Physics*, 9: 546538, 2021.

17. C D Aiello, D D Awschalom, H Bernien, T Brower-Thomas, K R Brown, T A Brun, J R Caram, E Chitambar, R Di Felice, M F J Fox, S Haas, A W Holleitner, E R Hudson, J H Hunt, R Joynt, S Koziol, H J Lewandowski, D T McClure, J Palsberg, G Passante, K L Pudenz, C J K Richardson, J L Rosenberg, R S Ross, M Saffman, M Singh, D W Steuerman, C Stark, J Thijssen, A N Vamivakas, J D Whitfield, B M Zwickl. Achieving a Quantum Smart Workforce. *Quantum Science and Technology*, 6: 030501, 2021.

18. R Chien, J D Whitfield. Custom Fermionic Codes for Quantum Simulation. (Preprint) arXiv:2009.11860, 2020.

19. J D Whitfield. Understanding the Schrodinger Equation as a Kinematic Statement: A Probability-First Approach to Quantum. In "Understanding the Schrödinger Equation: Some [Non]Linear Perspectives"; Editors: V. A. Simpao, H. C. Little. Published by *Nova Publishers*, 2020.

20. Q Sun, X Zhang, S Banerjee, P Bao, M Barbry, N S Blunt, N A Bogdanov, G H Booth, J Chen, Z-H Cui, J J Eriksen, Y Gao, S Guo, J Hermann, M R Hermes, K Koh, P Koval, S Lehtola, Z Li, J Liu, N Mardirossian, J D McClain, M Motta, B Mussard, H Q Pham, A Pulkin, W Purwanto, P J Robinson, E Ronca, E Sayfutyarova, M Scheurer, H F Schurkus, J E T Smith, C Sun, S N Sun, S Upadhyay, L K Wagner, X Wang, A White, James Daniel Whitfield, M J Williamson, S Wouters, J Yang, J M Yu, T Zhu, T C Berkelbach, S Sharma, A Sokolov, G K-L Chan. Recent Developments in the PySCF Program Package. *Journal of Chemical Physics*, 153: 024109, 2020.

21. K Setia, R Chien, J E Rice, A Mezzacapo, M Pistoia, J D Whitfield. Reducing Qubit Requirements for Quantum Simulation using Molecular Point Group Symmetries. *Journal of Chemical Theory and Computation*, 16 (10): 60916097, 2020.

22. J Brown, J Yang, J D Whitfield. Solver for the Electronic V-Representation Problem of Time-Dependent Density Functional Theory. *Journal of Chemical Theory and Computation*, 16 (10): 6014-6026, 2020.

23. K Setia, S Bravyi, A Mezzacapo, J D Whitfield. Superfast Encodings for Fermionic Quantum Simulation. *Physical Review Research*, 1: 033033, 2019.

24. S Gulania, J D Whitfield. Young Frames for Quantum Chemistry. (Preprint) arXiv: 1904.10469.

25. R W Chien, S Xue, T S Hardikar, K Setia, J D Whitfield. Analysis of Superfast Encoding Performance for Electronic Structure Simulations. *Physical Review A*, 100: 032337, 2019.

26. J Brown, J D Whitfield. Basis Set Convergence of Wilson Basis Functions for Electronic Structure. *Journal of Chemical Physics*, 151: 064118, 2019.

27. K Setia, J D Whitfield. Bravyi-Kitaev Superfast Simulation of Fermions on a Quantum Computer. *The Journal of Chemical Physics*, 148: 164104, 2018.

28. C Schilling, M Altunbulak, S Knecht, A Lopes, J D Whitfield, M Christandl, D Gross, M Reiher. Generalized Pauli Constraints in Small Atoms. *Physical Review A*, 97: 052503, 2018.

29. G Zhu, Y Subasi, J D Whitfield,, M Hafezi. Hardware-Efficient Fermionic Simulation with a Cavity-QED System. *New Physics Journal Quantum Information*, 4: 16, 2018.

30. V Havlíček, M Troyer, J D Whitfield. Operator Locality in Quantum Simulation of Fermionic Models. *New Physics Journal Quantum Information*, 95: 032332, 2017.

31. J D Whitfield, V Havlíček, M Troyer. Local Spin Operators for Fermion Simulations. *Physical Review A*, 94: 030301, 2016.

32. S Barz, B Dakic, Y O Lipp, F Verstraete, J D Whitfield, P Walther. Linear-Optical Generation of Eigenstates of the Two-Site XY Model. *Physical Review X*, 5(2): 021010, 2015.

33. Y Wang, F Dolde, J Biamonte, R Babbush, V Bergholm, S Yang, I Jakobi, P Neumann, A Aspuru-Guzik, J D Whitfield, and J Wrachtrup. Quantum Simulation of Helium Hydride Cation in a Solid-State Spin Register. *ACS Nano*, 9(8): 7769-7774, 2015.

34. J D Whitfield, M-H Yung, D G Tempel, S Boixo, A Aspuru-Guzik. Computational Complexity of Time-Dependent Density Functional Theory. *New Journal of Physics*, 16(8): 083035, 2014.

35. J D Whitfield, Z Zimborás. On the NP-Completeness of the Hartree-Fock Method for Translationally Invariant Systems. *The Journal of Chemical Physics*, 141(23): 234103, 2014.

36. J D Whitfield. Communication: Spin-Free Quantum Computational Simulations and Symmetry Adapted States. *The Journal of Chemical Physics*, 139: 021105, 2013.

37. J D Whitfield, P J Love, and A Aspuru-Guzik. Computational Complexity in Electronic Structure. *Physical Chemistry Chemical Physics*, 15(2): 397-411, 2013.

38. Z Zimboras, M Faccin, Z Kadar, J D Whitfield, B Lanyon, and J Biamonte. Quantum Transport Enhancement by Time-Reversal Symmetry Breaking. *Scientific Reports*, 3: 2361, 2013.

39. J D Whitfield, M Faccin, and J D Biamonte. Ground-State Spin Logic. *EPL (Europhysics Letters)*, 99(5): 57004, 2012.

40. N C Jones, J D Whitfield, P L McMahon, M-H Yung, R Van Meter, A Aspuru-Guzik, and Y Yamamoto. Faster Quantum Chemistry Simulation on Fault-Tolerant Quantum Computers. *New Journal of Physics*, 14(11): 115023, 2012.

41. I Kassal, J D Whitfield, A Perdomo-Ortiz, M-H Yung, and A Aspuru-Guzik. Simulating Chemistry Using Quantum Computers. *Annual Review of Physical Chemistry*, 62: 185-207, 2011.

42. J D Whitfield, J Biamonte, and A Aspuru-Guzik. Simulation of Electronic Structure Hamiltonians Using Quantum Computers. *Molecular Physics*, 109(5): 735-750, 2011.

43. J D Biamonte, V Bergholm, J D Whitfield, J Fitzsimons, and A Aspuru-Guzik. Adiabatic Quantum Simulators. *AIP Advances*, 1(2): 022126-022126, 2011.

44. Z Li, M-H Yung, H Chen, D Lu, J D Whitfield, X Peng, A Aspuru-Guzik, and J Du. Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance. *Scientific Reports*, 1: 2011.

45. B P Lanyon, J D Whitfield, G G Gillett, M E Goggin, M P Almeida, I Kassal, J D Biamonte, M Mohseni, B J Powell, M Barbieri, et al. Towards Quantum Chemistry on a Quantum Computer. *Nature Chemistry*, 2(2): 106-111, 2010.

46. M-H Yung, D Nagaj, J D Whitfield, and A Aspuru-Guzik. Simulation of Classical Thermal States on a Quantum Computer: A Transfer-Matrix Approach. *Physical Review A*, 82(6): 060302, 2010.

47. J D Whitfield, C A Rodriguez-Rosario, and A Aspuru-Guzik. Quantum Stochastic Walks: A Generalization of Classical Random Walks and Quantum Walks. *Physical Review A*, 81(2): 022323, 2010.

Other Works

1. C Dowdle and J D Whitfield. A Practical Introduction to Quantum Computing. Link to SIAM News. May 1, 2024.

2. J D Whitfield, S Hassinger, and Z Mohammad. Introducing the Amazon Braket Learning Plan and Digital Badge. Link to blogpost, November 27, 2023.

3. K Setia, J D Whitfield, and T Takeshita. Bernoulli line and the Bloch sphere: visualizing probability and quantum states. Link to blogpost, December 23, 2022.

4. J D Whitfield. Sprinternships with Break Through Tech Chicago and the Amazon Braket quantum computing team. Link to blogpost, December 21, 2022.

5. Z Mohammad, C Madsen, and J D Whitfield. Introducing the Amazon Braket Algorithm Library. Link to blogpost. November 28, 2022.

Press and Other Items

- Dartmouth Communications Office
  - *2024 Summer Term Highlights*. Professor J.D. Whitfield Link to video, August 29, 2024.
  - *Faculty Expert Series*. Professor J D Whitfield on What Muons Are and What They Do.Link to video, June 2, 2021.
  - C Albright. From Zeros and Ones to Qubits: Teaching Quantum Computing. Link to article, February 2, 2020.
  - J. Blumberg. At Dartmouth Computing With the Experts. Link to article, February 24, 2019.
- Newspaper coverage and podcasts
  - A Manning. Uncovering "hidden curriculum" for those historically on outside Quantum Noir fosters sense of community amount individuals of color interest or involved in quantum science, nanoscience, engineering. Link to article, June 21, 2024.
  - K Rowney and S Hassinger (hosts). Probability First: Understanding Quantum Computing with J D Whitfield. *The New Quantum Era Podcast*. Link to podcast, April 10, 2023.
  - S Earle. Future Problem Solvers. *Valley News.* Link to article, November 2, 2020.
  - With computing, Dartmouth is thinking very, very small. *Concord Monitor*. Link to article, February 2, 2019.
  - D Brooks. Dartmouth is Doubling Down on Quantum Computing. *Concord Monitor*. Link to article, January 23, 2019.
  - M Golec. Leaping into Quantum Computing. *Valley News*. Link to article, January 26, 2019.
- Amazon Science
  - D Gantenbein. A Conversation With J D Whitfield, Amazon Visiting Academic on Quantum Computing. Link to blogpost. July 16, 2021.