

James Brown

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Education

PhD , Physics, Queen's University, Kingston, ON, Canada	2016
MSc , Physics, Queen's University, Kingston, ON, Canada	2012
BSc , Physics, minor in Economics, McMaster University, Hamilton, ON, Canada	2010

Research Experience

Department of Physics and Astronomy, Dartmouth College, Hanover, NH, 2017-present

Postdoctoral research conducted with Dr. James Whitfield

Using grid-based methods to solve for electronic energies and densities with a focus on applications to quantum computers. One published paper. One paper submitted. One paper in preparation.

Department of Chemistry, Temple University, Philadelphia, PA, 2016-2017

Postdoctoral research conducted with Dr. Spiridoula Matsika

Developed a fully quantum method to analyse vibrations after the radiationless decay of a molecule through a conical intersection.

Department of Physics, Engineering Physics & Astronomy, Queen's University, Kingston, ON, 2012-2016

Doctoral thesis research conducted with Dr. Tucker Carrington Jr.

Improved the performance of phase-space motivated basis sets when applied to calculating vibrational energies of molecules. Four published papers.

Department of Physics, Engineering Physics & Astronomy, Queen's University, Kingston, ON, 2010-2012

Masters' thesis research conducted with Dr. Tucker Carrington Jr.

Applied previously developed numerical methods to calculate rovibrational energies of molecules.

Developed new model to analyse oddities in calculated values. Four published papers of which one was an Editors' Choice.

Department of Physics and Astronomy, McMaster University, Hamilton, ON, 2009-2010

Honor's thesis research conducted with Dr. Dmitry Pelinovsky.

Studied computational methods that obtain numerical solutions to the nonlinear Schrodinger equation.

Science Department, Redeemer University College, Hamilton, ON, 2008-2009

Undergraduate summer research conducted with Dr. Wytse van Dijk and Dr. Kyle Spyksma

Implemented and evaluated the accuracy and efficiency of numerical solutions to the time-dependent Schrodinger equation. Resulted in one publication.

Publications

James Brown, Jun Yang and James D. Whitfield, "Solver for the electronic V-representation problem of time-dependent density functional theory", (submitted to J. Chem. Theory Comput.)

James Brown and James D. Whitfield, "Basis set convergence of Wilson basis functions for electronic structure", J. Chem. Phys., 2019, 151(6), 064118

James Brown and Tucker Carrington Jr., "Using an expanding nondirect product harmonic basis with an iterative eigensolver to compute vibrational energy levels with as many as seven atoms", J. Chem. Phys., 2016, 145(14), 144104

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James Brown and Tucker Carrington Jr., "Assessing the utility of phase-space-localized basis functions: exploiting direct product structure and a new basis function selection procedure", J. Chem. Phys., 2016, 144(24), 244115

A McKellar, M. Dehghany, Mojtaba Rezaei, N. Moazzen-Ahmadi, **James Brown**, Xiao-Gang Wang, Tucker Carrington "Intermolecular vibrations of the CO₂ - CS₂ complex: Experiment and theory agree, but understanding remains challenging", J. Mol. Spectrosc. 2016 (in press)

James Brown and Tucker Carrington Jr., "Using an iterative eigensolver to compute vibrational energies with phase-spaced localized basis functions", J. Chem. Phys., 2015, 143(04), 044104

James Brown and Tucker Carrington Jr., "Comment on "Phase-Space Approach to Solving the Time-Independent Schrödinger Equation"", Phys. Rev. Lett., 2015, 114(05), 058901

James Brown, Xiao-Gang Wang, Tucker Carrington Jr., G.S. Grubbs II, and Richard Dawes, "Computational study of the rovibrational spectrum of CO₂-CS₂", J. Chem. Phys., 2014, 140(11), 114303, (J. Chem. Phys Editors' Choice for 2014)

James Brown, Xiao-Gang Wang, and Tucker Carrington Jr., "Calculating and assigning rovibrational energy levels of (¹⁵N₂O)₂, (¹⁵N¹⁴N₂O)₂, ¹⁴N₂O-¹⁵N₂O and ¹⁵N¹⁴N₂O-¹⁵N₂O", Phys. Chem. Chem. Phys., 2013, 15(44), 19159-19168

James Brown, Xiao-Gang Wang, Richard Dawes, and Tucker Carrington Jr., "Computational study of the rovibrational spectrum of (OCS)₂", J. Chem. Phys., 2012, 136(13), 134306

Wytse van Dijk, **James Brown** and Kyle Spyksma, "Efficiency and accuracy of numerical solutions to the time-dependent Schrödinger equation", Physical Review E, 2011, 84(5), 056703

Talks

"The Wilson basis applied to electronic structure", 2018 Symposium on Chemical Physics, University of Waterloo, Nov 2-4, 2018

"Improving the efficiency of phase-space localized basis functions", Exploiting New Advances in Mathematics to Improve Calculations in Quantum Molecular Dynamics, Banff International Research Station, January 24-29, 2016

"Computing the vibrational energies of CH₂O and CH₃CN with phase-space localized functions and an iterative eigensolver", 71st International Symposium on Molecular Spectroscopy, University of Illinois Champaign-Urbana, June 20-24, 2015

"Calculating and assigning rovibrational energies of four N₂O dimer isotopologues", 2013 Symposium on Chemical Physics, University of Waterloo, Nov 1-3, 2013

"Computation of the rovibrational spectra of Van der Waal complexes and their isotopologues", 5th Annual Queen's Chemistry Graduate Symposium, Queen's University, Sept 7, 2012

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"The dynamics of the OCS dimer and a new cross-shaped structure", 2011 Symposium on Chemical Physics, University of Waterloo, Nov 4-6, 2011

Poster Presentations

"Phase-space localized basis functions applied to sum-of-products potentials", 2015 Symposium on Chemical Physics, University of Waterloo, Nov 6-8, 2015

"Calculating rovibrational energies using phase-space localized basis functions in polyspherical coordinates", 2014 Symposium on Chemical Physics, University of Waterloo, Nov 7-9, 2014

"The application of phase-space localized basis functions to the calculation of rovibrational energies in polyspherical coordinates", 26th Canadian Symposium on Theoretical and Computational Chemistry, Concordia University, July 6-11, 2015

"Computational study of the rovibrational spectrum of CO₂-CS₂: Evidence of Internal Rotation", 2012 Symposium on Chemical Physics, University of Waterloo, Nov 2-4, 2012

"Computational study of the rovibrational spectrum of CO₂-CS₂: Evidence of Internal Rotation", Vibrational Spectroscopy, University of New England, Aug 5-10, 2012

Scholarships

- **Ontario Graduate Scholarship**, one year, merit based, Queen's University 2015-2016
- **Queen Elizabeth II Graduate Scholarship in Science and Technology**, one year, merit based, Queen's University 2014-2015
- **Duncan & Urrla Carmichael Graduate Fellowship**, one year, merit based, Queen's University 2013-2014
- **R.S. McLaughlin Fellowship**, two years, merit based, Queen's University 2010-2012
- **NSERC Undergraduate Student Research Award**, Redeemer University, 2010
- **Industrial NSERC Undergraduate Student Research Award**, Integrity Testing Laboratories Inc., 2008

Teaching Experience

Department of Physics, Engineering Physics & Astronomy, Queen's University, Kingston

Teaching assistant for PHYS/ENPH 312 Mathematical Methods in Physics 2013-2016

Teaching assistant for PHYS 117 Introductory Physics 2012-2013

Teaching assistant for PHYS 104/106 Fundamental Physics 2010-2012