GRIER MAXIMILLIAN JONES, PHD

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RESEARCH INTERESTS

Chemistry	Inorganic, physical, computational and theoretical chemistry
Mathematics	Topological data analysis, graph theory, ordinary and partial differential equations, optimization, dynamical systems, and mathematical modeling
Computer Science	High performance computing, quantum computing, cloud computing, machine learning, acceleration hardware (GPUs, TPUs, etc.)

EDUCATION

Feb. 1, 2024-Present	**Postdoctoral Fellow** The Edward S. Rogers Sr. Department of Electrical Engineering and Computer Engineering University of Toronto, Toronto, ON, CA Department of Chemical and Physical Sciences University of Toronto Mississauga, Mississauga, ON, CA Quantum Software Consortium, CA Advisors: Dr. H.-A. Jacobsen, Dr. U. Fekl
Aug. 1, 2018-Dec. 16, 2023	**PhD in Physical Chemistry** **Interdisciplinary Graduate Minor in Computational Sciences (IGMCS)** Department of Chemistry University of Tennessee, Knoxville, TN, USA Advisor: Dr. K. D. Vogiatzis
Sept. 2014-May 12, 2018	**BS in Chemistry (American Chemical Society Certified)** **Minor in Mathematics** Department of Chemistry and Biochemistry College of Charleston, Charleston, SC, USA Advisors: Dr. P. Riggs-Gelasco, Dr. W. G. Mitchener, Dr. G. A. Guirgis

CONTINUING EDUCATION AND PROFESSIONAL DEVELOPEMENT

May 2024-June 2025	Prospective Professors in Training Program at the University of Toronto
July 15-26, 2024	2024 Qiskit Global Summer School: The Path to Utility Additional Certificates: Badge of Quantum Excellence
June 22/27-29, 2022	San Diego Supercomputer Center Cyberinfrastructure-Enabled Machine Learning Summer Institute
September 4, 2019	OMSC Workshop at EUCO-CTC 2019, Perugia, Italy
December 10-13, 2018	34th Annual Winter School in Theoretical Chemistry 2018: Machine Learning in Theoretical Chemistry (Helsinki)

WORK EXPERIENCE

Feb. 2024- **Postdoctoral Fellow at the University of Toronto, St. George and Mississauga Campuses, ON, CA**

- Experience developing quantum machine learning and distributed quantum algorithms using common Python quantum computing packages, such as Qiskit and Pennylane, on IBM hardware

- Experience running quantum chemical calculations on high performance computing platforms using Gaussian
- Decommissioned an outdated server and assisted in the construction and commissioning of a new group cloud server
- Worked in a highly collaborative environment, which includes the mentorship of undergraduate and master's students
- Participated as a program committee member to peer-review papers, schedule talks, and run the discussion session for a conference workshop on distributed quantum computing
- Assisted in writing proposals and grants, along with participating in group recruitment activities, such as interviewing potential undergraduate candidates
- Published conference workshop papers, one peer-review journal article, with other manuscripts in preparation to be submitted to peer-reviewed journals
- Helped organize a workshop on distributed quantum computing at IEEE Quantum Week 2024, 2025, and 2026
- Lead a collaborative project with an industrial partner
- Represented the Quantum Software Consortium in meetings with industry partners and collaborators

Jan. 2019-Jan. 2024 **Graduate Research Assistant at the University of Tennessee, Knoxville, TN**

- Worked on the development of data-driven quantum chemistry approaches using common Python machine learning packages such as scikit-learn, PyTorch, and Deep Graph Library
- Experience running quantum chemical calculations on high performance computing platforms using OpenMolcas, Psi4/Psi4Numpy, TURBOMOLE, and ORCA
- Successful utilization of tools based on topological data analysis, including persistent homology, for chemical applications related to electronic structure theory, catalysis, and polymer dynamics
- Worked in a highly collaborative environment and mentored six undergraduate researchers on various research projects
- Published four first author peer-reviewed journal articles, along with a book and book chapter with code examples available in public repositories
- Received recognition via national and departmental awards, along with regional, national, and international presentations

Aug. 2018-Dec. 2021 **Graduate Teaching Assistant at the University of Tennessee, Knoxville, TN**

- Responsibilities included grading exams and assignments, creating assignments, tutorial center hours, and teaching laboratory and discussion sessions
- During COVID-19 this introduced new challenges and responsibilities such as online and hybrid teaching, writing exam questions, and online proctoring
- Gained experience with course planning by helping pioneer the first course on machine learning in chemistry in the Department of Chemistry

May 2015-May 2018 **Undergraduate Research Assistant at the College of Charleston, Charleston, SC**

- Developed machine learning models for image generating tasks related to hallucinations and mental imagery using Mathematica
- Implemented mathematical models using Mathematica for the study of chaos in parametric resonance optical/acoustical diffraction experiments
- Received two poster awards for the best poster presentations from the Department of Mathematics
- Worked with collaborators at the Medical University of South Carolina and in the Department of Physics at the College of Charleston
- Performed optimization and frequency quantum chemical calculations, in the Department of Chemistry and Biochemistry, using Gaussian

Summer 2012	**National Park Service Youth Corp member, Kings Mountain National Military Park, Blacksburg, SC** • Maintained trails, built bridges in remote locations, assisted in efforts to maintain fire lines for seasonal controlled burns, and performed routine maintenance on park equipment

TEACHING EXPERIENCE

March 13 & 16, 2026	Quantum Information Processing: Algorithms & Software (ECE484; guest lecturer) University of Toronto, St. George
Fall 2025-Winter 2026	Modular Quantum Computing Algorithms for Quantum Chemistry (PHY479Y) University of Toronto, St. George
Summer 2025	Optimizing Quantum Chemistry Calculations using Quantum Machine Learning Methods (PHY479Y) University of Toronto, St. George
Fall 2024	Quantum Machine Learning Architecture Searches for Chemical Application (CSC495H1) University of Toronto, St. George
Fall 2021	Special Topics in Chemistry II: Machine Learning for Chemical Applications (CHEM 420) University of Tennessee, Knoxville
Spring 2021	Foundations of Physical Chemistry (CHEM 370) University of Tennessee, Knoxville
Spring 2020	General Chemistry II (CHEM 130) University of Tennessee, Knoxville
Fall 2018, Spring 2019, Fall 2019, Fall 2020	General Chemistry I (CHEM 120) University of Tennessee, Knoxville

PEER-REVIEWED ARTICLES

Exploring Transferability of Quantum Machine Learning Methods in Quantum Chemical Applications, *In Preparation.*
G. Holmen, **G. M. Jones**, V. K. Prasad

Trainable Pulse Encoder and Progressive Circuit Growth for Quantum Machine Learning, *In Preparation.*
T. Trenty, **G. M. Jones**, V. K. Prasad, H.-A. Jacobsen

Leveraging Data-Driven Coupled-Cluster to Initialize the Local Unitary Cluster Jastrow Ansatz, *In Preparation.*
M. Leach, M. Amoussou, **G. M. Jones**, H.-A. Jacobsen

Quantum Machine Learning for Transition Metal Catalysis: Accelerating C-H Activation Pathway Design, *In Preparation.*
G. M. Jones, C. Liu, I. González Valenzuala, U. Fekl, H.-A. Jacobsen

Large-scale Electronic Structure Calculations Utilizing Distributed Quantum-centric Supercomputing, *In Preparation.*
J. R. Moore, A. K. Rao, I. Shezad, S. J. Wagner, **G. M. Jones**, H.-A. Jacobsen

Probabilistic Design of Parametrized Quantum Circuits through Local Gate Modifications, *Submitted.*
G. M. Jones, A. Newatia, A. Lao, A. K. Rao, V. K. Prasad, H.-A. Jacobsen

Parametrized Quantum Circuit Learning for Quantum Chemical Applications, *J. Chem. Inf. Model., **2026**, 2026, 66, 6, 3103–3116.*
G. M. Jones, V. K. Prasad, U. Fekl, H.-A. Jacobsen

Capturing Electron Correlation with Machine Learning through a Data-Driven CASPT2 Framework, *J. Chem. Theory Comput.,* 2025, 21, 21, 10879–10892.
G. M. Jones, K. D. Vogiatzis

Analyzing Common Electronic Structure Theory Algorithms for Distributed Quantum Computing, In *2025 IEEE International Conference on Quantum Computing and Engineering (QCE)*, 2025, 368-373.
G. M. Jones, H.-A. Jacobsen

In Silico Screening of CO_2-Dipeptide Interactions for Bioinspired Carbon Capture, *ChemPhysChem,* 2024, e202400498
A. G. Sylvanus, **G. M. Jones**, R. Custelcean, K. D. Vogiatzis

Distributed Quantum Computing for Chemical Applications, In *2024 IEEE International Conference on Quantum Computing and Engineering (QCE*), 2024, Vol. 2, 155-160.
G. M. Jones, H.-A. Jacobsen

Data-Driven Refinement of Electronic Energies from Two-Electron Reduced-Density-Matrix Theory. *J. Phys. Chem. Lett.*, 2023, 14, 28, 6377-6385.
G. M. Jones, R. R. Li, A. E. DePrince III, K. D. Vogiatzis

Data-Driven Ligand Field Exploration of Fe(IV)-oxo Sites for C-H Activation. *Inorg. Chem. Front.*, 2023, 10, 1062-1075. (Featured on front cover)
G. M. Jones, B. A. Smith, J. K. Kirkland, K. D. Vogiatzis

BOOKS

Molecular Representations for Machine Learning, ACS In Focus Series, 2023.
G. M. Jones, B. Story, V. Maroulas, K. D. Vogiatzis

BOOK CHAPTERS

Data-driven acceleration of coupled-cluster and perturbation theory methods, in: "Quantum Chemistry in the Age of Machine Learning", Editor: Pavlo Dral, Elsevier, 2023. 509-529.
G. M. Jones, P. D. V. S. Pathirage, K. D. Vogiatzis

JOURNALS REVIEWED

Summer 2025	IEEE Transactions on Networking
Summer 2025	2025 IEEE International Conference on Quantum Computing and Engineering (QCE)
Summer 2024	2024 IEEE International Conference on Quantum Computing and Engineering (QCE)

RESEARCH PRESENTATIONS

Talks

February 20, 2026	Quantum Days 2026, Victoria, CA: *Quantum Consortia Presentation – QSC: Unlocking Distributed Quantum Computing for Canada* **(Invited)**
February 18, 2026	Quantum Days 2026, Victoria, CA: *Panel Session – Distributed Quantum Computing: Toward Error-Corrected, Scalable Quantum Systems* **(Invited)**
November 19, 2025	2025 Maryland Delegation to University of Toronto and CQIQC **(Invited)**
October 21, 2025	Ontario Public Service Share Your Science 2025: Uncertainty, Imagination, Impact: Science

	at the Edge of Change: *Panel Discussion on Quantum Science* **(Invited)**
October 21, 2025	Ontario Public Service Share Your Science 2025: Uncertainty, Imagination, Impact: Science at the Edge of Change: *The Quantum Software Consortium of Canada: Exploring Distributed Quantum Solutions for Canada* **(Invited)**
September 4, 2025	WKS38—Distributed Quantum Computing: Applications, Challenges and Opportunities at the IEEE International Conference on Quantum Computing and Engineering (QCE), Albuquerque, New Mexico, USA: *Analyzing Common Electronic Structure Theory Algorithms for Distributed Quantum Computing*
July 11, 2025	Quantum Software Consortium 2025 Annual General Meeting: *Pushing quantum chemistry beyond classical limitations using distributed quantum computing*
June 11, 2025	University of Tennessee, Chattanooga, USA: *Pushing quantum chemistry beyond classical limitations using distributed quantum computing* **(Invited)**
May 23, 2025	Two Small Fish Ventures: *Crash Course on Quantum Computing* **(Invited)**
September 29, 2024	Q-SITE, Toronto, CA: *Distributed Quantum Computing for Chemical Applications* **(Invited)**
September 18, 2024	WKS19—Distributed Quantum Computing Algorithms, Networks, Software, and Applications at the IEEE International Conference on Quantum Computing and Engineering (QCE), Montreal, CA: *Distributed Quantum Computing for Chemical Applications*
August 17, 2023	Machine Learning in Chemistry session at the American Chemical Society, San Francisco, USA: *Exploring the Topology of Electron Correlation with Graph Neural Networks*
May 12, 2023	Southeastern Theoretical Chemistry Association Meeting (SETCA) 2022, South Carolina, USA: *Exploring the Topology of Electron Correlation with Graph Neural Networks*
September 4, 2019	Open Molecular Science Cloud (OMSC) Workshop at EUCO-CTC 2019, Perugia, Italy: *Data-driven Quantum Chemistry with Cloud Computing*
November 17, 2017	College of Charleston Mathematics Colloquium: *Simulating an Acoustical Experiment*
November 4, 2016	College of Charleston Mathematics Colloquium: *A Mathematical Model of Dynamic Vision*
September 25, 2015	College of Charleston Mathematics Colloquium: *Modeling Mental Imagery*

Posters

July 11, 2025	Quantum Software Consortium 2025 Annual General Meeting, Toronto, CA: *Understanding Parameterized Quantum Circuit Learning for Chemical Applications*
February 19, 2025	Quantum Days 2025, Toronto, CA: *A Combinatorial Search of Parameterized Quantum Circuit Learning for Chemical Applications*
October 1, 2024	Data Sciences Institute Research Day 2024, the Data Sciences Institute, Toronto, CA: *Near-term Quantum Algorithms and Error Correction for Molecular Property Predictions*
August 28, 2024	10th International Conference on Quantum Information and Quantum Control (CQIQC-X), The Fields Institute, Toronto, CA: *Near-term Quantum Algorithms and Error Correction for*

	Molecular Property Predictions
March 28, 2023	NVIDIA GPU Award session at the American Chemical Society, Indianapolis, USA: *Exploring the Topology of Electronic correlation with Graph Neural Networks*
May 19, 2022	Southeastern Theoretical Chemistry Association Meeting (SETCA) 2022, Georgia Tech, USA: *Data-Driven Exploration of Fe(IV)-oxo Sites for C-H activation*
November 13, 2021	Symposium on Machine Learning in Quantum Chemistry (SMLQC-2021), online, Xiamen, China: *Data-Driven Accelerated Complete Active Space Second-Order Perturbation Theory*
April 12, 2018	College of Charleston School of Science and Mathematics 30th Annual Poster Session: *Simulating an Acoustical Experiment*
April 20, 2017	College of Charleston School of Science and Mathematics 29th Annual Poster Session: *A Mathematical Model of Dynamic Vision*
August 22, 2016	2016 Celebration of Scholars: Exposition of Faculty and Student Research, Scholarship, and Creativity: *A Mathematical Model of Dynamic Vision*
April 14, 2016	College of Charleston School of Science and Mathematics 28th Annual Poster Session: *Modeling Mental Imagery*
February 5, 2016	Medical University of South Carolina Neuroscience Institute Neuropalooza: *Modeling Mental Imagery*
August 28, 2015	MUSC Neuroscience Institute Meet & Greet Reception: *Modeling Mental Imagery*
August 24, 2015	2015 Celebration of Scholars: Exposition of Faculty and Student Research, Scholarship, and Creativity: *Modeling Mental Imagery*

AWARDS AND HONORS

April 1, 2024	Volunteer of Distinction, University of Tennessee
May 4, 2023	Gleb Mamantov Graduate Chemistry Scholar, Department of Chemistry, University of Tennessee
March 28, 2023	NVIDIA GPU Award for Best GPU Poster, COMP Division of the American Chemical Society
February 10, 2023	Graduate Student Senate Travel Award, University of Tennessee
September 2019	OMSC Workshop Travel Grant, Molecular Science Software Institute, NSF
April 12, 2018	Research Poster Session Award of Merit/Best Department of Mathematics Research Poster, College of Charleston School of Science and Mathematics 30th Annual Poster Session: *Simulating an Acoustical Experiment*
April 20, 2017	Research Poster Session Award of Merit/ Best Department of Mathematics Research Poster, College of Charleston School of Science and Mathematics 29th Annual Poster Session: *A Mathematical Model of Dynamic Vision*

PROFESSIONAL MEMBERSHIPS

2025-2026	Institute of Electrical and Electronics Engineers (IEEE)
2019-2026	American Chemical Society (ACS)

2016-2018	College of Charleston Math Club
2015-2018	Alpha Chi Sigma, Gamma Delta Chapter
Summer 2015	College of Charleston and Medical University of South Carolina Machine Learning and Medical Image Analysis Journal Club
Fall 2014	South Carolina Student Legislature

MENTORING

Summer 2025-	Maforikan Amoussou University of Toronto, St. George Campus
Summer 2025	Maximilian Leach University of Toronto, St. George Campus/University of Exeter Awards: 2025 MITACS Globalink Research Internship
Summer 2025	Ismael González Valenzuela University of Toronto, St. George Campus/National Autonomous University of Mexico Awards: 2025 MITACS Globalink Research Internship
Summer 2025-Winter 2026	Jenny Moore University of Toronto, St. George Campus Awards: CQIQC Undergraduate Summer Research Program 2025
Summer 2025	Liu Chen University of Toronto, St. George Campus/The Hong Kong Polytechnic University Awards: 2025 MITACS Globalink Research Internship
Fall 2024-Winter 2026	Adi Rao University of Toronto, St. George Campus
Fall 2024-Summer 2025	Aviraj Newatia University of Toronto, St. George Campus
Summer 2024	Alexander Lao University of Toronto, St. George Campus Awards: Engineering Science Research Opportunities Program (ESROP), University of Toronto
Summer 2024-Fall 2024	Logan Blaskie University of Toronto, Mississauga Campus Awards: 2024 University of Toronto Excellence Award (UTEA), University of Toronto
Summer 2024-Fall 2024	Andrew Jamsa University of Toronto, Mississauga Campus
Summer 2024	Kaalkidan Sahele University of Toronto, St. George Campus/Durham University Awards: 2024 MITACS Globalink Research Internship
Summer 2024	Thomas Trenty University of Toronto, St. George Campus/Bordeaux Institute of Technology Awards: 2024 MITACS Globalink Research Internship Master's Student

Fall 2023-January 2024	Amarachi G. Sylvanus University of Tennessee, Knoxville Graduate Student
Fall 2023-January 2024	Thomas Jones University of Tennessee, Knoxville Graduate Student
Fall 2019-January 2024	P. D. Varuna S. Pathirage University of Tennessee, Knoxville Graduate Student
Summer 2023-January 2024	Sean Liner University of Tennessee, Knoxville
Spring 2022-January 2024	Jacob Steeley University of Tennessee, Knoxville Awards: 2022 and 2023 Advanced Undergraduate Research Activity (AURA), University of Tennessee
Summer 2022-Spring 2023	Justin Phillips University of Tennessee, Knoxville
Spring 2022-Fall 2022	Carmen Brown University of Tennessee, Knoxville
Spring 2022	Zoe Edge University of Tennessee, Knoxville
Summer 2022	Catarus Hawkins University of Tennessee, Knoxville/Philander Smith College Awards: UT-Oak Ridge Innovation Institute Student Mentoring and Research Training (SMarT) program

SERVICE

Winter-Fall 2026	Technical Program Committee for the Quantum Machine Learning at 2026 IEEE International Conference on Quantum Computing and Engineering (QCE), Toronto, Ontario, CA
Winter-Fall 2026	Program committee member of the *Distributed Quantum Computing: Applications, Challenges And Opportunities* at 2026 IEEE International Conference on Quantum Computing and Engineering (QCE), Toronto, Ontario, CA
Winter-Fall 2026	2026 IEEE International Conference on Quantum Computing and Engineering (QCE) Student Volunteer Co-Chair, Toronto, Ontario, CA
September 4, 2025	Program committee member of the *Distributed Quantum Computing: Applications, Challenges And Opportunities* at 2025 IEEE International Conference on Quantum Computing and Engineering (QCE), Albuquerque, New Mexico, USA
September 18, 2024	Volunteer organizer for *Distributed Quantum Computing: Algorithms, Networks, Software, and Applications* at 2024 IEEE International Conference on Quantum Computing and Engineering (QCE), Montreal, Quebec, CA
March 3-4, 2023	Research Open House Host at the University of Tennessee, Knoxville
May 16-18, 2019	Volunteer at the 2019 Southeastern Theoretical Chemistry Association (SETCA) at the University of Tennessee, Knoxville

Fall 2017-Spring 2018	Co-Social Chair Executive Board Member, Alpha Chi Sigma, Gamma Delta Chapter
March 10, 2018	Alpha Chi Sigma Dance Volunteer at the 2018 MUSC Miracle Network Cougarthon
February 9, 2018	Alpha Chi Sigma Donut Fundraiser Volunteer for the 2018 MUSC Miracle Network Cougarthon
October 19, 2017	Hanahan Elementary School Family Science Night Magic Show
August 2017	Higdon Student Leadership Center Cougar Excursion Peer Facilitator
Fall 2016-Spring 2017	Executive Board Member, Alpha Chi Sigma, Gamma Delta Chapter
March 25, 2017	Water Mission International 2017 Charleston Walk for Water
March 2017	College of Charleston Accepted Students Weekend volunteer
February 18, 2017	Alpha Chi Sigma chemistry magic show volunteer at the 2017 MUSC Miracle Network Dance Marathon
September 10, 2016	Alpha Chi Sigma chemistry magic show volunteer at the Boeing Company annual luncheon held at North Charleston Riverfront Park
August 2016	Higdon Student Leadership Center Cougar Excursion Peer Facilitator
March 2016	College of Charleston Accepted Students Weekend volunteer
February 27, 2016	Alpha Chi Sigma chemistry magic show volunteer at the 2016 MUSC Miracle Network Dance Marathon
February 27, 2016	College of Charleston Mathematics Department Math Meet volunteer
October 23, 2015	Alpha Chi Sigma chemistry magic show volunteer at local homeschool association STEM fair, Calvary Lutheran Church, West Ashley, SC
October 1, 2015	2015 Preservation Society of Charleston Fall Tour of Homes Docent for 8 Legare Street, Charleston, SC
August 2015	Higdon Student Leadership Center Cougar Excursion Peer Facilitator
April 3, 2015	Alpha Chi Sigma fundraiser volunteer for the Shifa Clinic Child Hunger Prevention Program
March 2015	College of Charleston Accepted Students Weekend volunteer
February 18, 2015	Alpha Chi Sigma chemistry magic show volunteer at the 2015 MUSC Miracle Network Dance Marathon
Fall 2014	South Carolina Student Legislature Semi-Annual State House Session Delegate
August 2014	Higdon Student Leadership Center Cougar Excursion participant

ADDITIONAL SKILLS

Programming Languages	Python, FORTRAN, Mathematica, Bash and Zsh
Software and APIs	Git, CMake, Make

Professional Tools	LaTeX, ChemDraw, Microsoft Office Suite, VIM/VI
Computational Chemistry Software	Gaussian, MOLCAS/OpenMOLCAS, ORCA, TURBOMOLE, and Psi4/Psi4Numpy
High Performance Computing	Experience using high-performance computing (HPC) environments with schedulers such as Portable Batch System (PBS) and Simple Linux Utility for Resource Management (SLURM)
Operating Systems	Mac, Linux (Debian, Fedora, Ubuntu), Microsoft (includes setting up the Ubuntu Linux subsystem for Windows)
Professional Conduct	Completed Collaborative Institutional Training Initiative Program Physical Science Responsible Conduct of Research Course
Language	Basic knowledge in French.
Administration	Former manager of the lab Slack, OpenMOLCAS build, and system administrator for the network-attached storage (QNAP model type).