

Daniel Gibney

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About

Quantum Chemist/Software Engineer with 7 years of experience using Python/C++ for quantum chemistry, developing physics-based simulations of chemical systems to accurately elucidate molecular properties. A published record of success using convex optimization for improved molecular predictions at lower computational cost. Experienced in automating calculations using Python and bash scripting on high-performance computers for high-throughput data collection and post-processing. A leader with extensive experience bridging communications between disparate groups and finding common ground. Collaborative team player with a demonstrated passion for solving problems and excitement for tackling new opportunities in both industry and academia.

Education

- PhD** **The University of Chicago**, Chemistry Chicago, IL
 Sept 2019 – Aug 2024
- Thesis: Transformation of Density Functional Theory (DFT) into a 1-Electron Reduced Density Matrix Functional Theory (RDMFT) for the Treatment of Strong Correlation
 - Advisor: Prof. David Mazziotti
 - Freud Fellowship Award Recipient for Outstanding Scientific Achievement
- BS** **Florida State University**, Computer Science and Chemistry Tallahassee, FL
 Sept 2015 – May 2019
- Thesis: Finite Jellium Models for Plasmonic Nano-Particles
 - Advisor: Prof. Eugene DePrince
 - Cum Laude

Experience

- University of Minnesota**, Postdoctoral Scholar Minneapolis, MN
 Aug 2024 – present
 1 year 9 months
- Theory Development
 - Successfully demonstrated DFA 1-RDMFT's utility in [Fe-S] clusters, enabling large, difficult systems to be accurately studied at low cost
 - Optimized DFA 1-RDMFT specific properties enabling black-box utility for simplified user adoption
 - Developed an open-source parallel Python implementation of the Anti-hermitian Contracted Schrödinger Equation for highly accurate simulations of quantum systems
 - Collaborations
 - Led efforts with synthetic chemists to produce models connecting chemical properties with experimentally observed reactivity
 - Automated high-throughput calculations (6000+) and data collection to identify synthetically promising targets to optimize experimental efforts
 - 6 Publications
 - 4 First-authorships
- University of Chicago**, Graduate Research Assistant Chicago, IL
 Aug 2019 – Aug 2024
 5 years 1 month
- Developed a novel hybrid density functional and reduced density matrix functional method for the accurate simulation of strongly correlated molecules
 - Volunteered as a Director of Graduate Student Initiatives where I spearheaded efforts to improve the experience of graduate students
 - Mentored junior graduate and undergraduate students in quantum chemistry topics
 - 5 first-author publications

University of Chicago , Graduate Teaching Assistant	Chicago, IL
<ul style="list-style-type: none"> • Led general chemistry and undergraduate quantum mechanics discussion sections to facilitate student understanding • Directed general chemistry lab sections to ensure student learning and safety • Responsible for the grading of student lab reports, homeworks, and exams 	Aug 2019 – May 2020 10 months
Florida State University , Research Assistant	Tallahassee, FL
<ul style="list-style-type: none"> • Developed a C++ Psi4 Plugin for modeling plasmonic nanoparticles • Updated existing GPU accelerated code to maintain package compatibility 	Aug 2017 – May 2019 1 year 10 months
Florida State University , Laboratory Assistant	Tallahassee, FL
<ul style="list-style-type: none"> • Set up and tore down weekly general chemistry lab classes • Assisted students and teaching assistants when lab issues arose • Facilitated a legally blind student in their general chemistry laboratory work 	Aug 2017 – May 2019 1 year 10 months

Projects

ACSE	Aug 2025 – present
<p>An open-source implementation of the anti-Hermitian contracted Schrödinger equation for electronic ground and excited states</p> <ul style="list-style-type: none"> • Spin blocked for efficient computation with no loss in accuracy • Highly accurate absolute and relative energetics on par with or exceeding the traditional MRPT results • No dependence on the active space size enabling systems previously intractable to standard techniques 	
DFA 1-RDMFT	Aug 2019 – present
<p>A hybrid DFT and 1-RDMFT method for the accurate simulation of large, strongly correlated molecules</p> <ul style="list-style-type: none"> • Low computational scaling equal to the density functional approximation used • Equal treatment of strong and weak correlation in molecular systems • Available in the Maple Quantum Chemistry Package 	
Crystal Field Theory Viewer	Jan 2023 – present
<p>Website for 3D visualization of d orbital splitting due to ligand coordination</p> <ul style="list-style-type: none"> • On device 3D rendering of accurate 3d orbitals and their energy level splittings under customizable ligand geometries and strengths • Built using Tailwind and Plotly 	
Visual-SCF	2025 – present
<p>Visual programming package for teaching and learning quantum chemistry</p> <ul style="list-style-type: none"> • Python-based gui for quantum chemistry programming and learning 	
Etsy-Workflow-Accelerator	2025 – present
<p>GUI Python application for quickly converting and sorting PDFs into PNGs for Etsy listings</p> <ul style="list-style-type: none"> • Automatic folder structure generation • Mass ingest and conversion of PDFs to PNGs 	

Publications

Open-source implementation of the anti-Hermitian contracted Schrödinger equation for electronic ground and excited states	Under review
<p><i>Daniel Gibney</i>, Anthony W. Schlimgen, Jan-Niklas Boyn 10.48550/arXiv.2604.02550 (arXiv)</p>	

<p>Holistic Simulation of Iron-Sulfur Cluster Electronic and Physical Structures with Hybrid Density Functional Approximation Reduced Density Matrix Functional Theory <i>Daniel Gibney</i>, Shelby T. Davis, Jan-Niklas Boyn 10.26434/chemrxiv.10001732/v1 (ChemRxiv)</p>	Under review
<p>Disentangling Cooperative Electron Correlation and Primary Coordination Sphere Effects in [4Fe-4S]⁺ Structural Isomerism and π-Acid Activation Shelby T. Davis, <i>Daniel Gibney</i>, Jan-Niklas Boyn 10.1021/acs.jpcllett.5c03723 (The Journal of Physical Chemistry Letters)</p>	Feb 2026
<p>Myriad aryne derivatives from carboxylic acids Chris M. Seong, Sallu S. Kargbo, Chia-Ling Yu, <i>Daniel Gibney</i>, Jan-Niklas Boyn, Courtney C. Roberts 10.1038/s41586-025-09830-1 (Nature)</p>	Jan 2026
<p>Tunable Aromaticity and Biradical Character in Tetrathiafulvalene and Tetraselenafulvalene Derivatives <i>Daniel Gibney</i>, Jan-Niklas Boyn 10.1021/acs.jpca.5c05283 (The Journal of Physical Chemistry A)</p>	Sept 2025
<p>Benchmarking and Contrasting Exchange–Correlation Functional Differences in Response to Static Correlation in Unrestricted Kohn–Sham and a Hybrid 1-Electron Reduced Density Matrix Functional Theory <i>Daniel Gibney</i>, Jan-Niklas Boyn 10.1021/acs.jctc.5c00244 (Journal of Chemical Theory and Computation)</p>	May 2025
<p>Enhancing density-functional theory for static correlation in large molecules <i>Daniel Gibney</i>, Jan-Niklas Boyn, David Mazziotti 10.1103/PhysRevA.110.L040802 (Physical Review A)</p>	Oct 2024
<p>Universal generalization of density functional theory for static correlation <i>Daniel Gibney</i>, Jan-Niklas Boyn, David Mazziotti 10.1103/PhysRevLett.131.243003 (Physical Review Letters)</p>	Dec 2023
<p>Comparison of Density-Matrix Corrections to Density Functional Theory <i>Daniel Gibney</i>, Jan-Niklas Boyn, David Mazziotti 10.1021/acs.jctc.2c00625 (Journal of Chemical Theory and Computation)</p>	Oct 2022
<p>Density functional theory transformed into a one-electron reduced-density-matrix functional theory for the capture of static correlation <i>Daniel Gibney</i>, Jan-Niklas Boyn, David Mazziotti 10.1021/acs.jpcllett.2c00083 (The Journal of Physical Chemistry Letters)</p>	Feb 2022
<p>Toward a resolution of the static correlation problem in density functional theory from semidefinite programming <i>Daniel Gibney</i>, Jan-Niklas Boyn, David Mazziotti 10.1021/acs.jpcllett.0c03371 (The Journal of Physical Chemistry Letters)</p>	Dec 2020

Skills

Languages: Python, C++

Software, Tools, and Libraries: Orca, PySCF, Gaussian, Psi4, NumPy, SciPy, CVXPY, Matplotlib, Pandas, Plotly

Research Areas: Density Functional Theory, Reduced Density Matrix Functional Theories, Strong Correlation, Reaction Pathways, Model Generation

Presentations

- Application and Development of Quantum Chemical Methods - University of Minnesota Duluth 2026
- Application and Development of Quantum Chemical Methods - Saint Mary's 2026
- Transformation of DFT into a DFA 1-RDMFT for the capture of static correlation - ByteDance 2025
- Density Functionals in a 1-Electron Reduced Density Matrix Theory Framework - Toward a Solution to the Static Correlation Error - APS 2025
- Pursuit of Strongly Correlated Electrons on Classical and Quantum Devices - ACS Joint Midwest & Great Lakes Regional Meeting 2023
- Density Functional Theory Transformed into a One-Electron Reduced Density-Matrix Functional Theory for the Capture of Strong Correlation - ACS Fall 2022