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 Achievment

BS **Florida State University**, Computer Science and Chemsitry — Tallahassee, Florida — Sept 2015 – May 2019

- Thesis: Finite Jellium Models for Plasmonic Nano-Particles
- Cum Laude

Experience

University of Minnesota, Postdoctoral Scholar — Chicago, IL — 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 parallelized Python implementation of the Anti-hermitian Contracted Schrodginer Equation for highly accurate simulations of quantum systems
- Collaborations
- Lead efforts with synthetic chemists to produce models to connect chemical properties with experimentally observed reactivity
- High-throughput calculations (6000+) to identify synthetically promising targets to optimize experimental efforts
- 5 papers
- 3 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
- Published 5 first author papers

Florida State University, Research Assistant — Tallahassee, FL — Aug 2017 – May 2019 — 1 year 10 months

- Developed a C++ Psi4 Plugin for modeling plasmonic nanoparticles
- Updated existing gpu accelarated code to maintain package compatibility

Florida State University, Laboratory Assistant — Tallahassee, FL
- Set up and torn down weekly general chemisty lab classes — Aug 2017 – May 2019
- Assisted students and teaching assistants when lab issues arose — 1 year 10 months

Florida State University, General Chemistry Facilitator — Tallahasse, Fl
- Facilitated a legally blind student in their general chemistry laboratory work — Aug 2018 – Dec 2018, 5 months

Projects

DFA 1-RDMFT — Aug 2019 – present

A hybrid DFT and 1-RDMFT method for the accurate simulation of large, strongly correlated molecules
- Low computational scaling equal to the density functional approximation used
- Equal treatment of strong and weak correlation in molecular systems

Crystal Field Theory Viewer — Jan 2023 – present

Website for 3D visualization of d orbital splitting due to ligand coordination
- On device 3D rendering of accurate 3d orbitals and their energy level splittings with customizable ligand geometries and strengths
- Built using tailwind and Plotly

Visual-SCF — 2025 – present

Visual programming package for teaching and learning quantum chemistry
- Python based gui for qm programming

Etsy-Workflow-Accelerator — 2025 – present

GUI Python application for quickly converting and sorting PDFs into PNGs for etsy listings
- Automatic folder structure generation
- Mass ingest and conversion of PDFs to PNGs

Publications

Holistic Simulation of Iron-Sulfur Cluster Electronic and Physical Structures with Hybrid Density Functional Approximation Reduced Density Matrix Functional Theory
Daniel Gibney, Shelby T. Davis, Jan-Niklas Boyn

Disentangling Cooperative Electron Correlation and Primary Coordination Sphere Effects in [4Fe-4S]+ Structural Isomerism and π-Acid Activation — Jan 2026
Shelby T. Davis, *Daniel Gibney*, Jan-Niklas Boyn
10.26434/chemrxiv-2025-jg1qj-v2 (ChemRxiv)

Myriad aryne derivatives from carboxylic acids — Jan 2026
Chris M. Seong, Sallu S. Kargbo, Chia-Ling Yu, *Daniel Gibney*, Jan-Niklas Boyn, Courtney C. Roberts
10.1038/s41586-025-09830-1 (Nature 2026)

Tunable Aromaticity and Biradical Character in Tetrathiafulvalene and Tetraselenafulvalene Derivatives — Sept 2025
Daniel Gibney, Jan-Niklas Boyn
10.1021/acs.jpca.5c05283 (The Journal of Physical Chemistry A)

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 — May 2025
Daniel Gibney, Jan-Niklas Boyn
10.1021/acs.jctc.5c00244 (Journal of Chemical Theory and Computation)

Enhancing density-functional theory for static correlation in large molecules Oct 2024
Daniel Gibney, Jan-Niklas Boyn, David Mazziotti
10.1103/PhysRevA.110.L040802 (Physical Review A)

Universal generalization of density functional theory for static correlation Dec 2023
Daniel Gibney, Jan-Niklas Boyn, David Mazziotti
10.1103/PhysRevLett.131.243003 (Physical Review Letters)

Comparison of Density-Matrix Corrections to Density Functional Theory Oct 2022
Daniel Gibney, Jan-Niklas Boyn, David Mazziotti
10.1021/acs.jctc.2c00625 (Journal of Chemical Theory and Computation)

Density functional theory transformed into a one-electron reduced-density-matrix functional theory for the capture of static correlation Feb 2022
Daniel Gibney, Jan-Niklas Boyn, David Mazziotti
10.1021/acs.jpclett.2c00083 (The Journal of Physical Chemistry Letters)

Toward a resolution of the static correlation problem in density functional theory from semidefinite programming Dec 2020
Daniel Gibney, Jan-Niklas Boyn, David Mazziotti
10.1021/acs.jpclett.0c03371 (The Journal of Physical Chemistry Letters)

Skills

Languages: Python, C++

Softwares: 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

Talks

4. Transformation of DFT into a DFA 1-RDMFT for the capture of static correlation - ByteDance 2025
3. Density Functionals in a 1-Electron Reduced Density Matrix Theory Framework - Toward a Solution to the Static Correlation Error - APS 2025
2. Pursuit of Strongly Correlated Electrons on Classical and Quantum Devices - ACS Joint Midwest & Great Lakes Regional Meeting 2023
1. Density Functional Theory Transformed into a One-Electron Reduced Density-Matrix Functional Theory for the Capture of Strong Correlation ACS Fall 2022