Daniel Gibney

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ABOUT

Computational chemist with 5 years of experience developing physics-based simulations of chemical systems to accurately elucidate molecular structures and properties. A published record of success on combining reduced density matrices with density functionals for improved molecular predictions at lower computational cost. A leader with extensive experience in 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

University of Chicago Chicago, IL

PhD, M.S. in Chemistry Expected May 2024

- Honors: Freud Fellowship Award Recipient for Outstanding Scientific Achievement
- Thesis: Transformation of Density Functional Theory into a 1-Electron Reduced Density Matrix Functional Theory

Florida State University Tallahassee, FL

B.S. in Computer Science and Chemistry May 2019

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

SKILLS

Programming	Python, Bash, C/C++, HPC/Slurm, Basic JavaScript, Basic HTML/CSS
Software	PySCF, SciPy, Numpy, MatPlotLib, Anaconda, Maple, Quantum Chemistry Toolbox, CVXPY, LaTeX, three.js, pandas
Quantum Simulations	Ground state properties (Geometry Optimizations, Atomization Energies, Bond Enthalpies), Excited state properties (Vertical Excitation Energies, Oscillator Strengths, Real Time Propagations)
Websites	www.crystalfieldtheory.com, www.dpgibney.com (Hosted on AWS)

RESEARCH EXPERIENCE

University of Chicago Department of Chemistry Chicago, IL

Graduate Student with Dr. David Mazziotti August 2019 – Present

- Developing a novel RDMFT theory for strongly correlated electrons at low computational cost using reduced density matrices and semidefinite programming techniques
- Benchmarking RDMFT on 83 different test suites of chemical systems and properties
- Identifying functional driven vs density driven errors in RDMFT
- Building Python code to rapidly prototype new RDMFT algorithms and workflows

- Optimized RDMFT parameters to identify generalizable trends in reproducing potential energy surfaces
- Elucidated theoretical connections between related methodologies such as iDMFT and TAO-DFT

Florida State University Department of Chemistry Tallahassee, FL
Undergraduate Student with Dr. Eugene DePrince August 2017 - May 2019

- Developed a methodology using Particle In a Box wavefunctions for modeling Plasmonic Nanoparticles
- Investigated excited state properties of the model system using Real-Time Hartree Fock and Configuration Interaction Singles
- Exploited symmetry to significantly reduce computational time and memory requirements

PUBLICATIONS

Gibney, D., Boyn, J. and Mazziotti, D. (2023). *Universal Generalization of Density Functional Theory for Static Correlation.*

- Derived the RDMFT w value as a function of the 2-electron integrals for molecule specificity

Gibney, D., Boyn, J. and Mazziotti, D. (2022). *Comparison of Density-Matrix Corrections to DFT.*

- Quadratic RDMFT is related to the fermi-dirac distribution and Von-Neumann entropy
  The Quadratic RDMFT w value is dependent on the amount of Hartree-Fock exchange

Gibney, D., Boyn, J. and Mazziotti, D. (2022). *Density Functional Theory Transformed into a One-Electron Reduced-Density-Matrix Functional Theory for the Capture of Static Correlation.*

- A quadratic semi-definite program based on 1-RDM's captures static correlation effects

Gibney, D., Boyn, J. and Mazziotti, D. (2020). *Towards a Resolution of the Static Correlation Problem in Density Functional Theory from Semidefinite Programming.*

- Fractional occupations in degenerate frontier orbitals results in a variationally lower energy

PRESENTATIONS

- **Gibney, D**. *Density functional theory transformed into a one-electron reduced density-Matrix functional theory for the capture of static correlation.* Presented at the Fall 2022 American Chemical Society Meeting.
- **Gibney, D**. Schouten, A. Mazziotti, D. *Pursuit of strongly correlated electrons on classical and quantum devices*. Presented at the 2023 American Chemical Society Joint Midwest & Great Lakes Regional Meeting.

TEACHING EXPERIENCE

Quantum Mechanics: CHEM 261 Chicago, IL
Teaching Assistant October 2022 – December 2022

- Held weekly office hours; graded weekly problem sets, midterm exams, and final
- Responded to students emails to improve their understanding of lectures and homework
- Created detailed answer keys for all problems sets

- Class size: 63, 1 TA

General Chemistry: CHEM 111,112,113 Chicago, IL

Teaching Assistant August 2019 – June 2020

- Taught general chemistry students in weekly recitations, labs, and office hours
- Created practice problem sets to aid in students' understanding of general chemistry
- Graded problems sets, lab reports, and exams
- Class size: 200 students, 12 TAs

LEADERSHIP EXPERIENCE

University of Chicago Department of Chemistry Chicago, IL

Director of Graduate Student Initiatives July 2022 - July 2023

- Collaborated with a team of 3 other directors to organize monthly social events with members of the chemistry department ranging from small get togethers to large, 150+ people events
- Facilitated student and faculty discussions for better communication within the department and improved support for new graduate students

Epsilon Sigma Alpha, co-ed Service Fraternity Tallahassee, FL

VP of Recruitment August 2015 – June 2019

- Served as the Vice President of Recruitment for the 2016-2017 school year
- Volunteered weekly in and around Tallahassee through community gardens and neighborhood cleanups
- Raised funds for St. Jude Children's Hospital and spread awareness of their work

Florida State University Department of Chemistry Tallahassee, FL

Facilitator January 2017 – May 2017

- Assisted a legally blind student through their general chemistry lab course
- Responsible for ensuring safe laboratory etiquette and procedures
- Provided accurate chemical measurements when necessary