

Anderson D. S. Duraes

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EDUCATION

Ph.D. in Chemistry, **University of Notre Dame** August 2023
Department of Chemistry & Biochemistry Notre Dame, IN
Dissertation: *Enantiomeric Separation and the Hydrodynamic Properties of Chiral Molecules*
DOI: [10.7274/kp78gf09z02](https://doi.org/10.7274/kp78gf09z02)
Advisor: Dr. J. Daniel Gezelter (December 2018 – Present)
Dr. John Parkhill (June 2017 – July 2018)

B.S. in Chemistry, **Universidade Estadual de Campinas (UNICAMP)** July 2014
Additional Coursework in Advanced Mathematics Campinas, SP, Brazil
Exchange Program at Siena College (Loudonville, NY) through the Brazil Science Without Borders Undergraduate Program (Scholarship), Inducted into the Pi Mu Epsilon (U.S. Honorary National Mathematics Society) in 2013, Siena College President's List (Fall 2012 and Spring 2013)

RESEARCH EXPERIENCE

University of Notre Dame Notre Dame, IN
Graduate Research Assistant, Department of Chemistry and Biochemistry December 2018 – Present

- Investigating the separation of enantiomers without any chemical reactions using low-Reynolds number hydrodynamics and reverse non-equilibrium molecular dynamics (RNEMD)
- Employing hydrodynamics to study the transport properties of chiral and achiral swimmers

University of Notre Dame Notre Dame, IN
Graduate Research Assistant, Department of Chemistry and Biochemistry June 2017 – July 2018

- Applied restricted Boltzmann machine (RBM) to compress Slater determinants of the full configuration interaction (FCI) wavefunction
- Generated accurate potential energy surfaces (PES) for BeH₂, C₂, N₂ and F₂ using RBM

TEACHING EXPERIENCE

University of Notre Dame Notre Dame, IN
Teaching Assistant, Department of Chemistry and Biochemistry August 2017 – May 2020

- CHEM 30322: Conducted office hours to help students solve homework problems, graded homework and exams for a second-semester physical chemistry course
- CHEM 10171: Led tutorial sessions for 15-20 students, graded homework and exams for a first-year general chemistry course with a total enrollment of over 1000 students
- CHEM 11171 and CHEM 21274: Assisted students in experiments, laboratory techniques and graded lab reports for first- and second-year general chemistry laboratories

SKILLS

Languages: Portuguese (native speaker), English (proficient), French (intermediate level B1)

Computer: Python, Linux-/Unix-based computer systems, C, C++, LaTeX, Gaussian, GAMESS, PySCF, NWChem, Wolfram Mathematica, MATLAB, OpenOffice Math, OpenSCAD

Research: Strong analytical and problem-solving skills, Solid statistical skills, Multi-step synthesis, Essential laboratory procedures and Separation techniques, Analyze ^1H and ^{13}C NMR, IR and UV/Vis spectrometry

PUBLICATIONS

1. Anderson D. S. Duraes and J. Daniel Gezelter, “A Theory of Pitch for the Hydrodynamic Properties of Molecules, Helices, Propellers, and Achiral Swimmers”. Manuscript accepted for publication in *J. Chem. Phys.* (2023)
2. Anderson D. S. Duraes and J. Daniel Gezelter, “Separation of Enantiomers through Local Vorticity: A Screw Model Mechanism”, *J. Phys. Chem. B*, **125** (42), pp. 11709–11716 (2021); DOI: [10.1021/acs.jpcc.1c07127](https://doi.org/10.1021/acs.jpcc.1c07127); ChemRxiv: [10.33774/chemrxiv-2021-196zw](https://chemrxiv.org/abs/10.33774/chemrxiv-2021-196zw)
3. Anderson D. S. Duraes, “Compression of Exact Wavefunctions with Restricted Boltzmann Machine Auto-Encoders”; arXiv: [2304.00259](https://arxiv.org/abs/2304.00259)

PRESENTATIONS

1. *52nd Midwest Theoretical Chemistry Conference* June, 2022
The Ohio State University, Columbus, OH
Contributed Talk: “Separation of Enantiomers: A Screw Model Mechanism”
2. *2nd Annual Bay Area Chemistry Symposium* November 5, 2021
(Virtual event hosted by Gilead Sciences)
Poster Presentation: “Separation of Enantiomers: A Screw Model Mechanism”
3. *51st Midwest Theoretical Chemistry Conference* June 6–8, 2019
University of Notre Dame, Notre Dame, IN
Poster Presentation: “Enantiomers: Separation through Shear Vorticity”

REFERENCES

| Ph.D. advisor | Ph.D. committee member | Ph.D. committee member |
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| J. Daniel Gezelter Professor of Chemistry and Biochemistry, and Associate Dean College of Science University of Notre Dame (574) 631-7595 gezelter@nd.edu | Marya Lieberman Professor of Chemistry and Biochemistry University of Notre Dame (574) 631-4665 mlieberm@nd.edu | Steven Corcelli Professor of Chemistry and Biochemistry, and Department Chair University of Notre Dame (574) 631-2631 scorcell@nd.edu |