

Dominic A. Sirianni

DEPARTMENT OF NATURAL SCIENCES · DAEMEN UNIVERSITY

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Education

Georgia Institute of Technology (Advisor: C. David Sherrill)

Atlanta, GA

PH.D. IN PHYSICAL CHEMISTRY

2015–2020

Thesis Title: Electronic Structure Methods for Studying Non-Covalent Interactions in Complex Chemical Environments

Center for the Integration of Research, Teaching, & Learning

Atlanta, GA

CIRTL ASSOCIATE CERTIFICATE IN HIGHER EDUCATION

2018–2019

Edinboro University of Pennsylvania

Edinboro, PA

B.S. IN CHEMISTRY

2011–2015

Summa Cum Laude & Robert C. Weber Honors Program Graduate

Thesis Title: *Ab initio* study of 1,3,5-trihydroxy-1,3,5-triazin-2,4,6-[1H,3H,5H]-trione and its decomposition products

B.S. IN MATHEMATICS

2011–2015

Summa Cum Laude & Robert C. Weber Honors Program Graduate

Professional Experience

2022–	Assistant Professor of Chemistry Department of Natural Sciences, Daemen University	Amherst, NY
2020–'22	Postdoctoral Research Associate The Parish Lab: Gottwald Center for the Sciences, Department of Chemistry, University of Richmond	Richmond, VA
2016–'20	Graduate Research Assistant The Sherrill Group: Center for Computational Molecular Science and Technology, School of Chemistry & Biochemistry, Georgia Institute of Technology	Atlanta, GA
2016–'20	Systems Administrator The Sherrill Group: Center for Computational Molecular Science and Technology, School of Chemistry & Biochemistry, Georgia Institute of Technology	Atlanta, GA
2015–'16	Graduate Teaching Assistant School of Chemistry & Biochemistry, Georgia Institute of Technology	Atlanta, GA
2014	NSF REU Fellow The Sherrill Group: Center for Computational Molecular Science and Technology, School of Chemistry & Biochemistry, Georgia Institute of Technology	Atlanta, GA

Fellowships, Honors, & Awards

2019–'20	Larry S. O'Hara Fellowship (Top doctoral student in GT College of Sciences)	Atlanta, GA
2016	Honorable Mention NSF Graduate Research Fellowship Program	Atlanta, GA
2015–'19	President's Fellow Georgia Institute of Technology	Atlanta, GA

Publications

Undergraduate coauthors indicated with an asterisk ()*

13. Predicting the Barriers to Bergman-Type Cyclizations via Intramolecular Coulombic Repulsion

M. A. HENDLER,* A. BAKRY,* M. RAO,* J. E. AZAR-TANGUAY,* Z. CHEN,* S. A. MENDOZA-GOMEZ,* D. A. SIRIANNI, AND C. A. PARISH (*In preparation*)

12. An *Ab Initio* Study of the Diradical Isomers of Pyrrole, Furan, and Thiophene

J. E. AZAR-TANGUAY,* Z. CHEN,* S. A. MENDOZA-GOMEZ,* C. ANCAJAS,* D. A. SIRIANNI, AND C. A. PARISH (*In preparation*)

11. Variations on the Bergman Cyclization Theme: Electrocyclizations of Penta-, Hepta- and Octa-diyne

D. A. SIRIANNI, S. A. MENDOZA-GOMEZ,* X. SONG, S. WAIREGI,* M. FILATOV, E. B. WANG, A. LUXON,* M. ZIMMERLEY, A. NUSSDORF, R. HOFFMANN, AND C. A. PARISH (*In preparation*)

10. A Highly Correlated, Multireference Study of Aromatic Tetraradicals

D. A. SIRIANNI, J. B. SCHRIBER, T. A. GREENE* H. LISCHKA, AND C. A. PARISH (*In preparation*)

9. Building a Successful Computational Chemistry Laboratory

J. B. SCHRIBER, [D. A. SIRIANNI](#), G. FLANAGIN, C. A. PARISH, AND B. R. MILLER III, in *Physical Chemistry Research at Undergraduate Institutions: Innovative and Impactful Approaches, Volume 1*, C. A. PARISH AND T. A. HOPKINS Eds. 69-83 (2022) (doi: 10.1021/bk-2022-1428.ch005)

8. The influence of a solvent environment on direct non-covalent interactions between two molecules: A symmetry-adapted perturbation theory study of polarization tuning of π - π interactions by water

[D. A. SIRIANNI](#), X. ZHU, D. F. SITKOFF, D. L. CHENEY, AND C. D. SHERRILL, *J. Chem. Phys.* **156**, 19430 (2022) (doi: 10.1063/5.0087302)

7. Psi4Education: Free and Open-Source Programming Activities for Chemical Education with Free and Open-Source Software

D. B. MAGERS, V. H. CHÁVEZ, B. G. PEYTON, [D. A. SIRIANNI](#), R. C. FORTENBERRY, AND A. R. McDONALD, in *Teaching Programming across the Chemistry Curriculum*, A. R. McDONALD AND J. A. NASH Eds. 107-122 (2021) (doi: 10.1021/bk-2021-1387.ch008)

6. Optimized Damping Parameters for Empirical Dispersion Corrections to Symmetry-Adapted Perturbation Theory

J. B. SCHRIBER, [D. A. SIRIANNI](#), D. G. A. SMITH, L. A. BURNS, D. SITKOFF, D. L. CHENEY, AND C. D. SHERRILL, *J. Chem. Phys.* **154**, 234107 (2021) (doi: 10.1063/5.0049745)

5. Psi4 1.4: Open-Source Software for High-Throughput Quantum Chemistry

D. G. A. SMITH, L. A. BURNS, A. C. SIMMONETT, R. M. PARISH, M. C. SCHIEBER, R. GALVELIS, P. KRAUS, H. KRUSE, R. DI REMIGIO, A. ALENAIZAN, A. M. JAMES, S. LEHTOLA, J. P. MISIEWICZ, M. SCHEURER, R. A. SHAW, J. B. SCHRIBER, Y. XIE, Z. L. GLICK, [D. A. SIRIANNI](#), J. S. O'BRIEN, J. M. WALDROP, A. KUMAR, E. G. HOHENSTEIN, B. P. PRITCHARD, B. R. BROOKS, H. F. SCHAEFER III, A. Y. SOKOLOV, K. PATKOWSKI, A. E. DEPRINCE III, U. BOZKAYA, R. A. KING, F. A. EVANGELISTA, J. M. TURNEY, T. D. CRAWFORD, AND C. D. SHERRILL, *J. Chem. Phys.* **18**, 184108 (2020) (doi: 10.1063/5.0006002)

4. Tipping the Balance between S- π and O- π Interactions

J. WHANG, P. LI, M. D. SMITH, C. E. WARDEN, [D. A. SIRIANNI](#), E. C. VIK, J. M. MAIER, C. J. YEHL, C. D. SHERRILL, AND K. D. SHIMIZU, *J. Am. Chem. Soc.* **140**, 13301-13307 (2018) (doi: 10.1021/jacs.8b07617)

3. Psi4NUMPY: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development

D. G. A. SMITH, L. A. BURNS, [D. A. SIRIANNI](#), D. R. NASCIMENTO, A. KUMAR, A. M. JAMES, J. B. SCHRIBER, T. ZHANG, B. ZHANG, A. S. ABBOTT, E. BERQUIST, M. H. LECHNER, L. DOS A. CUNHA, A. G. HEIDE, R. A. KING, A. C. SIMMONETT, J. M. TURNEY, H. F. SCHAEFER, F. A. EVANGELISTA, A. E. DEPRINCE III, T. D. CRAWFORD, K. PATKOWSKI, AND C. D. SHERRILL, *J. Chem. Theory Comput.* **14**, 3504-3511 (2018) (doi: 10.1021/acs.jctc.8b00286)

2. Assessment of Density Functionals for Optimization of Bimolecular van der Waals Complexes

[D. A. SIRIANNI](#), A. ALENAIZAN, D. L. CHENEY, AND C. D. SHERRILL, *J. Chem. Theory Comput.* **14**, 3004-3013 (2018) (doi: 10.1021/acs.jctc.8b00114)

1. Comparison of Explicitly Correlated Methods for Computing High-Accuracy Benchmark Energies for Noncovalent Interactions

[D. A. SIRIANNI](#), L. A. BURNS, AND C. D. SHERRILL, *J. Chem. Theory Comput.* **13**, 86-99 (2017) (doi: 10.1021/acs.jctc.6b00797)

Presentations

CONTRIBUTED TALKS

A POGIL-Inspired Laboratory Exercise Deriving Reversibility of $P - V$ Work in a Simulated Ideal Gas

Virtual

[D. A. SIRIANNI](#)

November 2022

Lowering the Activation Barrier to Success in P-Chem (LABSIP) Fall 2022

A Highly Correlated, Multireference Study of Aromatic Tetraradicals

Atlanta, GA

[D. A. SIRIANNI](#) AND C. A. PARISH

August 2021

262nd National Meeting of the American Chemical Society

Variations on the Bergman cyclization theme: Electrocyclizations of Penta-, Hepta-, and Octadiynes

Virtual

[D. A. SIRIANNI](#) AND C. A. PARISH

April 2021

261st National Meeting of the American Chemical Society

PSI4EDUCATION: Leveraging “Dry” Technology as an Alternative to the Wet Chemistry Laboratory	<i>Virtual</i>
<u>D. A. SIRIANNI</u> 261st National Meeting of the American Chemical Society	<i>April 2021</i>
Improving Efficiency in Symmetry-Adapted Perturbation Theory	<i>Knoxville, TN</i>
<u>D. A. SIRIANNI</u> , D. G. A. SMITH, L. A. BURNS, D. SITKOFF, K. PATKOWSKI, D. L. CHENEY, AND C. D. SHERRILL 2019 Meeting of the Southeastern Theoretical Chemistry Association	<i>May 2019</i>
Improving Efficiency in Symmetry-Adapted Perturbation Theory	<i>Atlanta, GA</i>
<u>D. A. SIRIANNI</u> , D. G. A. SMITH, L. A. BURNS, D. SITKOFF, K. PATKOWSKI, D. L. CHENEY, AND C. D. SHERRILL 2019 Graduate Research Symposium, Georgia Tech School of Chemistry & Biochemistry Runner-Up: Outstanding Oral Presentation	<i>May 2019</i>
The Influence of Solvation on Non-Covalent Interactions in Bimolecular Complexes	<i>Banning Mills, GA</i>
<u>D. A. SIRIANNI</u> , X. ZHOU, D. SITKOFF, D. L. CHENEY, AND C. D. SHERRILL 2018 Graduate Research Retreat, Georgia Tech School of Chemistry & Biochemistry Winner: Outstanding Oral Presentation	<i>Oct 2018</i>
PSI4NUMPY: An Interactive Quantum Chemistry Programming Environment for Reference Implementation, Rapid Development, and Education	<i>Oxford, MS</i>
D. G. A. SMITH, <u>D. A. SIRIANNI</u> , L. A. BURNS, K. PATKOWSKI, AND C. D. SHERRILL 2017 Meeting of the Southeastern Theoretical Chemistry Association Winner: Outstanding Graduate Student Oral Presentation	<i>May 2017</i>
Comparison of Explicitly Correlated Methods for Computing High-Accuracy Benchmark Energies for Noncovalent Interactions	<i>Columbia, SC</i>
<u>D. A. SIRIANNI</u> , L. A. BURNS, AND C. D. SHERRILL 2016 Southeast Regional Meeting of the American Chemical Society	<i>Oct. 2016</i>
CONTRIBUTED POSTERS	
Variations on the Bergman Cyclization Theme: Electrocyclizations of Penta-, Hepta-, and Octa-diynes	<i>Blacksburg, VA</i>
<u>D. A. SIRIANNI</u> , S. A. MENDOZA-GOMEZ, AND C. A. PARISH 10th Triennial Conference on Molecular Quantum Mechanics	<i>June 2022</i>
Assessment of Density Functionals for Optimization of Bimolecular van der Waals Complexes	<i>Baton Rouge, LA</i>
<u>D. A. SIRIANNI</u> , A. ALENAIZAN, D. L. CHENEY, AND C. D. SHERRILL 2018 Meeting of the Southeastern Theoretical Chemistry Association	<i>May 2018</i>
PSI4NUMPY: An Interactive Quantum Chemistry Programming Environment	<i>New Orleans, LA</i>
D. G. A. SMITH, L. A. BURNS, <u>D. A. SIRIANNI</u> , D. R. NASCIMENTO, A. KUMAR, A. JAMES, J. SCHRIBER, T. ZHANG, B. ZHANG, A. ABBOTT, E. BERQUIST, M. LECHNER, L. DOS ANJOS CUNHA, A. SIMMONETT, J. TURNEY, F. EVANGELISTA, A. E. DEPRINCE III, T. D. CRAWFORD, K. PATKOWSKI, AND C. D. SHERRILL 255th National Meeting of the American Chemistry Society	<i>Mar. 2018</i>
Comparison of Explicitly Correlated Methods for Computing High-Accuracy Benchmark Energies for Noncovalent Interactions	<i>Tallahassee, FL</i>
<u>D. A. SIRIANNI</u> , L. A. BURNS, AND C. D. SHERRILL 2016 Meeting of the Southeastern Theoretical Chemistry Association	<i>May 2016</i>
Ab initio study of 1,3,5-trihydroxy-1,3,5-triazin-2,4,6[1H,3H,5H]-trione and its decomposition products	<i>San Francisco, CA</i>
<u>D. A. SIRIANNI</u> , N. D. KRAUT, N. KEBEDE, AND G. J. HOFFMAN 248th National Meeting of the American Chemical Society	<i>Aug. 2014</i>

Student Training

SIRIANNI LAB @ DAEMEN UNIVERSITY

2023– **Jillian E.-R. Baltzley** Undergraduate Student, Sirianni Lab
2023– **Kade Bidwell** Undergraduate Student, Sirianni Lab
2023– **Robert Horsmon** Undergraduate Student, Sirianni Lab
2023– **Aleksandr A. Selyuzhitskiy** Undergraduate Student, Sirianni Lab
2023 **Jonathan M. Berbert** Undergraduate Student, Sirianni Lab
2023 **Carlos H. Vargas III** Undergraduate Student, Sirianni Lab
2023 **Ryan M. Danzig** Undergraduate Student, Sirianni Lab
2023 **Marcelo Astudillo** Undergraduate Student, Sirianni Lab

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PARISH LAB @ THE UNIVERSITY OF RICHMOND

2022 **Marcos Hendler** Undergraduate Student, Parish Lab
2022 **Aamy Bakry** Undergraduate Student, Parish Lab
2022 **Maaz Rao** Undergraduate Student, Parish Lab
2021–'22 **Jean Azar-Tanguay** Undergraduate Student, Parish Lab
2021–'22 **Sebastian Mendoza-Gomez** Undergraduate Student, Parish Lab
2021–'22 **Charli Chen** Undergraduate Student, Parish Lab
2021–'22 **Mohamed Hussein** Undergraduate Student, Parish Lab
2020 **Salmika Wairegi** Undergraduate Student, Parish Lab

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SHERRILL GROUP @ GEORGIA TECH

2019–'20 **Derek Metcalf** First-Year Graduate Student & Systems
Administrator-In-Training, Sherrill Group
2016 **Constance Warden** First-Year Graduate Student, Sherrill Group
2016 **Seth Polansky** Georgia Tech REU Student

School of Chemistry & Biochemistry | Georgia Tech
School of Chemistry & Biochemistry | Georgia Tech
School of Chemistry & Biochemistry | Georgia Tech

Teaching Experience

INSTRUCTOR OF RECORD

Chemistry I

Department of Natural Sciences | Daemen University

CHE 110 (FIRST-YEAR UNDERGRADUATE LEVEL)

Fall '22, Spring '23

Course Description An introduction to the basic principles, theories and techniques of chemistry. Topics include stoichiometry, atomic structure, bonding, states of matter, equilibrium, thermodynamics, kinetics, electrochemistry and chemical reactions.

Chemistry II

Department of Natural Sciences | Daemen University

CHE 111 (FIRST-YEAR UNDERGRADUATE LEVEL)

Spring '23

Course Description A continuation of the study of the basic principles, theories and techniques of chemistry.

Biophysical Chemistry

Department of Natural Sciences | Daemen University

CHE 303/L (UPPER-DIVISION UNDERGRADUATE)

Fall '22

Course Description An introduction to biophysical chemistry including thermodynamics, chemical equilibrium, chemical kinetics, and quantum mechanics.

Mathematical Methods for Chemical Physics

School of Chemistry & Biochemistry | Georgia Tech

CHEM 6481/6491 R (UPPER-DIVISION UNDERGRADUATE/GRADUATE LEVEL)

Fall '16–'18

Course Description This course surveys mathematical concepts commonly encountered in chemical physics. Topics include complex analysis, linear algebra & functional analysis, statistics, ordinary & partial differential equations, and integral transformations.

Special Topics: Python for Data Science

School of Chemistry & Biochemistry | Georgia Tech

CHEM 4803/8843 DR (UPPER-DIVISION UNDERGRADUATE/GRADUATE LEVEL)

Fall '19

Course Description Students learn the basic principles of Data Science and develop skills working with the most common tools in the world of Data Science, building from foundational experience with computer programming in the highly versatile Python language. The knowledge and skills developed in this course will therefore be transferable directly to students' future careers in the science, technology, or business sectors.

Mentoring & Advising Experience

- 2018-'20 **Graduate Mentor** Small Group Leader & Program Co-Director: Graduate Mentorship Program *School of Chemistry & Biochemistry | Georgia Tech*
- 2016-'20 **First-Year Graduate Mentor** Panelist & Event Organizer: Graduate Mentorship Program *School of Chemistry & Biochemistry | Georgia Tech*

Professional Service & Societies

- 2022- **Faculty Member: Molecular Education and Research Consortium in Undergraduate Computational Chemistry (MERCURY)**
- 2018-'20 **Co-Director: Graduate Mentorship Program** *School of Chemistry & Biochemistry | Georgia Tech*
- 2018-'20 **Graduate Mentor** Small Group Leader & Program Co-Director: Graduate Mentorship Program *School of Chemistry & Biochemistry | Georgia Tech*
- 2016-'20 **First-Year Graduate Mentor** Panelist & Event Organizer: Graduate Mentorship Program *School of Chemistry & Biochemistry | Georgia Tech*
- 2018-'20 **Chair: Advisory Board, Graduate Student Forum** *School of Chemistry & Biochemistry | Georgia Tech*
- 2017-'19 **Student Representative: Graduate Curriculum Committee** *School of Chemistry & Biochemistry | Georgia Tech*
- 2016-'18 **President: Graduate Student Forum** *School of Chemistry & Biochemistry | Georgia Tech*
- 2016- **Member: Society for Industrial and Applied Mathematics**
- 2013- **Member: Pi Mu Epsilon National Mathematics Honor Society**
- 2013- **Member: American Chemical Society**