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*

  Graduated Summa Cum Laude with Honors
  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*

  Graduated Summa Cum Laude with Honors

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 graduate 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 (*)

12. **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. MENDOZA-GOMEZ,* D. A. SIRIANNI, AND C. A. PARISH *(In preparation)*

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

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

10. **Variations on the Bergman Cyclization Theme: Electrocyclizations of Penta–, Hepta– and Octa–diynes**

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

9. **A Highly Correlated, Multireference Study of Aromatic Tetraradicals**

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

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 Progamming 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. De-Prince 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 Optimzation 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 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   *Virtual*

D. A. Sirianni   *April 2021*

   261st National Meeting of the American Chemical Society

Improving Efficiency in Symmetry-Adapted Perturbation Theory   *Knoxville, TN*

D. A. Sirianni, D. G. A. Smith, L. A. Burns, D. Sitkoff, K. Patkowski, D. L. Cheney, and C. D. Sherrill   *May 2019*

   2019 Meeting of the Southeastern Theoretical Chemistry Association

Improving Efficiency in Symmetry-Adapted Perturbation Theory

Atlanta, GA

D. A. Sirianni, D. G. A. Smith, L. A. Burns, D. Sitkoff, K. Patkowski, D. L. Cheney, and C. D. Sherrill

May 2019

2019 Graduate Research Symposium, Georgia Tech School of Chemistry & Biochemistry
Runner-Up: Outstanding Oral Presentation

The Influence of Solvation on Non-Covalent Interactions in Bimolecular Complexes

Banning Mills, GA

D. A. Sirianni, X. Zhou, D. Sitkoff, D. L. Cheney, and C. D. Sherrill

Oct 2018

2018 Graduate Research Retreat, Georgia Tech School of Chemistry & Biochemistry
Winner: Outstanding Oral Presentation

Psi4NumPy: An Interactive Quantum Chemistry Programming Environment for Reference Implementation, Rapid Development, and Education

Oxford, MS

D. G. A. Smith, D. A. Sirianni, L. A. Burns, K. Patkowski, and C. D. Sherrill

May 2017

2017 Meeting of the Southeastern Theoretical Chemistry Association
Winner: Outstanding Graduate Student Oral Presentation

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

Columbia, SC

D. A. Sirianni, L. A. Burns, and C. D. Sherrill

Oct. 2016

2016 Southeast Regional Meeting of the American Chemical Society

Contributed Posters

Variations on the Bergman Cyclization Theme: Electrocyclizations of Penta-, Hepta-, and Octa-diynes

Blacksburg, VA

D. A. Sirianni, S. A. Mendoza-Gomez, and C. A. Parish

June 2022

10th Triennial Conference on Molecular Quantum Mechanics

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

Baton Rouge, LA

D. A. Sirianni, A. Alenaizan, D. L. Cheney, and C. D. Sherrill

May 2018

2018 Meeting of the Southeastern Theoretical Chemistry Association

Psi4NumPy: An Interactive Quantum Chemistry Programming Environment

New Orleans, LA

D. G. A Smith, L. A. Burns, D. A. Sirianni, 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

Mar. 2018

255th National Meeting of the American Chemistry Society

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

Tallahassee, FL

D. A. Sirianni, L. A. Burns, and C. D. Sherrill

May 2016

2016 Meeting of the Southeastern Theoretical Chemistry Association

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

San Francisco, CA

D. A. Sirianni, N. D. Kraut, N. Kebede, and G. J. Hoffman

Aug. 2014

248th National Meeting of the American Chemical Society

Student Training

2022–	**Marcos Hendler** Undergraduate Student, Parish Lab	*Department of Chemistry | University of Richmond*
2022–	**Aamy Bakry** Undergraduate Student, Parish Lab	*Department of Chemistry | University of Richmond*
2022–	**Maaz Rao** Undergraduate Student, Parish Lab	*Department of Chemistry | University of Richmond*
2021–	**Jean Azar-Tanguay** Undergraduate Student, Parish Lab	*Department of Chemistry | University of Richmond*
2021–	**Sebastian Mendoza-Gomez** Undergraduate Student, Parish Lab	*Department of Chemistry | University of Richmond*
2021–	**Charli Chen** Undergraduate Student, Parish Lab	*Department of Chemistry | University of Richmond*
2021–	**Mohamed Hussein** Undergraduate Student, Parish Lab	*Department of Chemistry | University of Richmond*
2020	**Salmika Wairegi** Undergraduate Student, Parish Lab	*Department of Chemistry | University of Richmond*
2019–'20	**Derek Metcalf** First-Year Graduate Student & Systems Administrator-In-Training, Sherrill Group	*School of Chemistry & Biochemistry | Georgia Tech*
2016	**Constance Warden** First-Year Graduate Student, Sherrill Group	*School of Chemistry & Biochemistry | Georgia Tech*
2016	**Seth Polansky** Georgia Tech REU Student	*School of Chemistry & Biochemistry | Georgia Tech*

Teaching Experience

INSTRUCTOR OF RECORD

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.
Duties Design course curriculum; write and lead course lectures; prepare assignments to augment classroom discussion; hold office hours to assist students with challenging concepts.

CO-INSTRUCTOR OF RECORD

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.
Duties Collaborate with co-instructor to design course curriculum; write and present course lectures; prepare projects and assignments to augment classroom discussion; hold office hours to assist students with challenging concepts.

SUBSTITUTE/GUEST LECTURER

Quantum Mechanics
School of Chemistry & Biochemistry \| Georgia Tech

CHEM 6491 (GRADUATE LEVEL) *Fall '16–'19*

Course Description Important concepts and applications of quantum mechanics at the intermediate level, including operators, perturbation and variational methods applied to atoms and molecules.
Duties Lead several 50-minute lectures to ∼15 graduate students, covering topics including the time independent Schrödinger equation, the postulates of quantum mechanics, the Dirac delta function and momentum space, and extensions of approximate methods to many electron systems.

Computational Chemistry
School of Chemistry & Biochemistry \| Georgia Tech

CHEM 6485 (GRADUATE LEVEL) *Spring '16–'20*

Course Description Introductory course in computational chemistry, discussing electronic structure theory, semiemphirical methods, molecular mechanics, transistion-state searching, and computation of thermodynamic quantities.
Duties Lead several 50-minute lectures to ∼25 graduate students, covering topics including the Born–Oppenheimer approximation and potential energy surfaces, the Hartree–Fock equations, basis sets, static and dynamical electron correlation, and molecular properties.

Physical Chemistry II
School of Chemistry & Biochemistry \| Georgia Tech

CHEM 3412 (UPPER-DIVISION UNDERGRADUATE LEVEL) *Spring '16*

Course Description Quantum mechanics, atomic and molecular structure, bonding theory, molecular spectroscopy, statistical mechanics.
Duties Lead two 50-minute lectures to ∼130 junior- and senior-level undergraduate students, covering topics including the ladder-operator solution to the quantum harmonic oscillator, degeneracy, and p-orbital splitting via the Stark effect.

Summary Data Science Bootcamp
Institute for Data Engineering and Science | Georgia Tech

IDEaS Bootcamp (Mixed Undergraduate/Graduate Level)   *Summer '19*

Course Description This one-week bootcamp provides undergraduate and graduate students in science and engineering who have an introductory-level familiarity with any computer programming language an introduction to data management and visualization, data modeling, deep learning, and scientific programming in the Python programming language.
Duties Lead one 30-minute lecture to a mixed audience of ∼80 undergraduate and graduate students covering the application of data science and deep learning to open research questions in the fields of quantum chemistry and electronic structure theory.

Summer Workshop in Data Science & Scientific Computing
Institute for Data Engineering and Science | Georgia Tech

IDEaS Workshop (Mixed Undergraduate/Graduate/Postgraduate Level)   *Summer '17–'18*

Course Description This five-week workshop engages undergraduates, graduate students, and postdocs/professionals in the comptational sciences, natural sciences, and engineering disciplines to provide an introduction to scientific computing and programming with emphasis on the topics of scientific computing using the Python programming language, numerical linear algebra, databases, and machine learning.
Duties Lead one 50-minute lecture to a mixed audience of ∼60 undergraduate, graduate, and professional students covering (i) variable scope and namespaces in the Python programming language and (ii) the basic functionality and usage of several advanced libraries for scientific computing in Python.

GRADUATE TEACHING ASSISTANT

Summer Data Science Bootcamp
Institute for Data Engineering and Science | Georgia Tech

IDEaS Bootcamp (Mixed Undergraduate/Graduate Level)   *Summer '19*

Duties Collaborate with instructors on developing interactive classroom activities and out-of-class assignemnts which target the students' development of desired knowledge and skills; lead classroom activities in interactive sessions; develop and implement virtual learning and collaboration environments for both students and instructors; provide targeted feedback to students on assignments via code review.

Summer Workshop in Data Science & Scientific Computing
Institute for Data Engineering and Science | Georgia Tech

IDEaS Workshop (Mixed Undergraduate/Graduate/Postgraduate Level)   *Summer '17–'18*

Duties Design collaborative classroom activities to augment lecture instruction; collaboratively write and grade out-of-class assignments and projects through code review, administrate online educational platforms and materials; coordinate with teaching assistants to ensure timely design of materials and feedback on assignments.

Physical Chemistry II
School of Chemistry & Biochemistry | Georgia Tech

CHEM 3412 (Upper-Division Undergraduate Level)   *Spring '16*

Course Description Quantum mechanics, atomic and molecular structure, bonding theory, molecular spectroscopy, statistical mechanics.
Duties Write and hold review sessions for each exam which highlight the important concepts and materials from the unit; hold office hours to assist students with specific course material; grade course homeworks, examinations, and projects; substitute lecturer.

General Chemistry I
School of Chemistry & Biochemistry | Georgia Tech

CHEM 1211K (First-Year Undergraduate Level)   *Fall '15*

Course Description Topics to be covered include atomic structure, bonding, properties of matter, thermodynamics and physical equilibria. Laboratory exercises supplement the lecture material.
Duties Lead two sections (24 students/section) in laboratory experiments; demonstrate and teach proper safety and laboratory technique; introduce and teach course content during pre-laboratory discussions; lead two sections (24 students/section) of recitation; hold individual tutoring hours to assist students with specific course material; grade laboratory reports, assignments, quizzes, and practical examinations.

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

2018–'20	**Co-Director: 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**	

Skills

Computational Chemistry Software	Psi4, Molpro, Q-CHEM, GAMESS, Gaussian, WebMO, IQMol, GaussView, Avogadro, PyMOL, VMD
Programming	Python, Bash/Shell, LaTeX, C/C++
Software Development	Git, GitHub, Open-Source Software Project Management

References

Carol Parish
Floyd D. and Elisabeth S. Gottwald
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University of Richmond
410 Westhampton Way
University of Richmond, VA, 23173
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C. David Sherrill
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School of Chemistry & Biochemistry
Georgia Institute of Technology
901 Atlantic Dr NW
Atlanta, GA 30332-0400
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Vasser Woolley Professor
School of Chemistry & Biochemistry
Georgia Institute of Technology
901 Atlantic Dr NW
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School of Chemistry & Biochemistry
Georgia Institute of Technology
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