Dominic A. **Sirianni**

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Education

Georgia Institute of Technology (Advisor: C. David Sherrill) — *Atlanta, GA*

Ph.D. in Physical Chemistry (ABD) — *2015–2020*

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

Doctoral Minor in Higher Education (in progress) — *2018–2020*

Center for the Integration of Research, Teaching, & Learning — *Atlanta, GA*

CIRTL Associate Cirtificate 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

2016–	**Graduate Research Assistant** The Sherrill Group: Center for Computational Molecular Science and Technology, School of Chemistry & Biochemistry, Georgia Institute of Technology	*Atlanta, GA*
2016–	**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*
2015	**Outstanding Department Senior** Department of Chemistry, Edinboro University of Pennsylvania	*Edinboro, PA*
2015	**Certificate of Merit** Department of Mathematics & Computer Science, Edinboro University of Pennsylvania	*Edinboro, PA*
2015	**Outstanding Service to the Department** Department of Chemistry, Edinboro University of Pennsylvania	*Edinboro, PA*
2015	**ACS Undergraduate Award in Inorganic Chemistry** Department of Chemistry, Edinboro University of Pennsylvania	*Edinboro, PA*
2013	**POLYED Undergraduate Award for Achievement in Organic Chemistry** Department of Chemistry, Edinboro University of Pennsylvania	*Edinboro, PA*
2011–'15	**Dean's List** College of Science and Health Professions, Edinboro University of Pennsylvania	*Edinboro, PA*
2011–'15	**Board of Governors Scholarship in Science and Mathematics** (Edinboro University of Pennsylvania's full-tuition merit scholarship)	*Edinboro, PA*

Publications

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 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)

Manuscripts in Preparation

2. **Optimized Damping Parameters for Empirical Dispersion Corrections to Symmetry-Adapted Perturbation Theory**
   D. A. Sirianni, D. G. A. Smith, L. A. Burns, D. F. Sitkoff, D. L. Cheney, and C. D. Sherrill *(In preparation)*
1. **The Influence of Solvation on Non-Covalent Interactions in Bimolecular Complexes: An Intramolecular Symmetry-Adapted Perturbation Study**
   D. A. Sirianni, X. Zhu, D. F. Sitkoff, D. L. Cheney, and C. D. Sherrill *(In preparation)*

Presentations

Invited Seminars & Colloquia

There and Back Again: A Quantum Chemist's Tale — *Edinboro, PA*
Alumni Seminar Series, Edinboro University of Pennsylvania — *Oct. 2018*

Mathematical Formalism of Modern Quantum Chemistry II: Approximate Methods — *Edinboro, PA*
Math & CS Research Colloquium, Edinboro Univeristy of Pennsylvania — *Oct. 2014*

Mathematical Formalism of Modern Quantum Chemistry I: Exact Solution of the Schrödinger Equation — *Edinboro, PA*
Math & CS Research Colloquium, Edinboro Univeristy of Pennsylvania — *Oct. 2014*

Comparison of Explicitly-Correlated Methods for Benchmarking Non-Covalent Interactions — *Edinboro, PA*
Undergraduate Research Colloquium, Department of Chemistry, Edinboro Univeristy of Pennsylvania — *Oct. 2014*

Contributed Talks

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 Meeting of the Southeast Regional Meeting of the American Chemical Society

Contributed Posters

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

2019–	**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, and prepare projects and assignments to augment classroo 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–'18*

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 '15–'19*

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 '15*

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.

Summer 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 '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 professionalstudents 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*

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 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 '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 Present a lecture with demonstrative code examples and lead one 50-minute lecture on advanced Python topics; design collaborative classroom activities to support lecture content and augment instruction; collaboratively write and grade out-of-class assignments and projects; 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–	**Graduate Mentor** Small Group Leader & Program Co-Director: Graduate Mentorship Program	*School of Chemistry & Biochemistry | Georgia Tech*
2016–	**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–	**Student Member: Society for Industrial and Applied Mathematics**	
2013–	**Student Member: Pi Mu Epsilon National Mathematics Honor Society**	
2013–	**Studen Member: American Chemical Society**	

Skills

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

References

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