

# Dominic A. Sirianni

SCHOOL OF CHEMISTRY & BIOCHEMISTRY · GEORGIA INSTITUTE OF TECHNOLOGY

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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

2016–	<b>Graduate Research Assistant</b> The Sherrill Group: Center for Computational Molecular Science and Technology, School of Chemistry & Biochemistry, Georgia Institute of Technology	Atlanta, GA
2016–	<b>Systems Administrator</b> The Sherrill Group: Center for Computational Molecular Science and Technology, School of Chemistry & Biochemistry, Georgia Institute of Technology	Atlanta, GA
2015–'16	<b>Graduate Teaching Assistant</b> School of Chemistry & Biochemistry, Georgia Institute of Technology	Atlanta, GA
2014	<b>NSF REU Fellow</b> 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	<b>Larry S. O'Hara Fellowship</b> (Top graduate student in GT College of Sciences)	Atlanta, GA
2016	<b>Honorable Mention</b> NSF Graduate Research Fellowship Program	Atlanta, GA
2015–'19	<b>President's Fellow</b> Georgia Institute of Technology	Atlanta, GA
2015	<b>Outstanding Department Senior</b> Department of Chemistry, Edinboro University of Pennsylvania	Edinboro, PA
2015	<b>Certificate of Merit</b> Department of Mathematics & Computer Science, Edinboro University of Pennsylvania	Edinboro, PA
2015	<b>Outstanding Service to the Department</b> Department of Chemistry, Edinboro University of Pennsylvania	Edinboro, PA
2015	<b>ACS Undergraduate Award in Inorganic Chemistry</b> Department of Chemistry, Edinboro University of Pennsylvania	Edinboro, PA
2013	<b>POLYED Undergraduate Award for Achievement in Organic Chemistry</b> Department of Chemistry, Edinboro University of Pennsylvania	Edinboro, PA
2011–'15	<b>Dean's List</b> College of Science and Health Professions, Edinboro University of Pennsylvania	Edinboro, PA
2011–'15	<b>Board of Governors Scholarship in Science and Mathematics</b> (Edinboro University of Pennsylvania's full-tuition merit scholarship)	Edinboro, PA

## Publications

### 5. PSI4 1.4: Open Source Software for High-Throughput Quantum Chemistry

D. G. A. SMITH, L. A. BURNS, A. C. SIMMONETT, R. M. PARRISH, 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. SCHRIEBER, 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. YU. 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.* (Submitted)

#### 4. Tipping the Balance between S— $\pi$ and O— $\pi$ 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. SCHRIEBER, 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 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)

## 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

ALUMNI SEMINAR SERIES, EDINBORO UNIVERSITY OF PENNSYLVANIA

Edinboro, PA

Oct. 2018

#### Mathematical Formalism of Modern Quantum Chemistry II: Approximate Methods

MATH & CS RESEARCH COLLOQUIUM, EDINBORO UNIVERSITY OF PENNSYLVANIA

Edinboro, PA

Oct. 2014

#### Mathematical Formalism of Modern Quantum Chemistry I: Exact Solution of the Schrödinger Equation

MATH & CS RESEARCH COLLOQUIUM, EDINBORO UNIVERSITY OF PENNSYLVANIA

Edinboro, PA

Oct. 2014

#### Comparison of Explicitly-Correlated Methods for Benchmarking Non-Covalent Interactions

UNDERGRADUATE RESEARCH COLLOQUIUM, DEPARTMENT OF CHEMISTRY, EDINBORO UNIVERSITY OF PENNSYLVANIA

Edinboro, PA

Oct. 2014

### CONTRIBUTED TALKS

#### Improving Efficiency in Symmetry-Adapted Perturbation Theory

D. A. SIRIANNI, 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

Knoxville, TN

May 2019

#### Improving Efficiency in Symmetry-Adapted Perturbation Theory

D. A. SIRIANNI, 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

Atlanta, GA

May 2019

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

D. A. SIRIANNI, 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

Banning Mills, GA

Oct 2018

## PSI4NUMPY: An Interactive Quantum Chemistry Programming Environment for Reference Implementation, Rapid Development, and Education

D. G. A. SMITH, D. A. SIRIANNI, L. A. BURNS, K. PATKOWSKI, AND C. D. SHERRILL

2017 Meeting of the Southeastern Theoretical Chemistry Association

**Winner:** Outstanding Graduate Student Oral Presentation

Oxford, MS

May 2017

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

D. A. SIRIANNI, L. A. BURNS, AND C. D. SHERRILL

2016 Meeting of the Southeast Regional Meeting of the American Chemical Society

Columbia, SC

Oct. 2016

## CONTRIBUTED POSTERS

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

D. A. SIRIANNI, A. ALENAIZAN, D. L. CHENEY, AND C. D. SHERRILL

2018 Meeting of the Southeastern Theoretical Chemistry Association

Baton Rouge, LA

May 2018

### PSI4NUMPY: An Interactive Quantum Chemistry Programming Environment

D. G. A. SMITH, L. A. BURNS, D. A. SIRIANNI, D. R. NASCIMENTO, A. KUMAR, A. JAMES, J. SCHRIEBER, 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

New Orleans, LA

Mar. 2018

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

D. A. SIRIANNI, L. A. BURNS, AND C. D. SHERRILL

2016 Meeting of the Southeastern Theoretical Chemistry Association

Tallahassee, FL

May 2016

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

D. A. SIRIANNI, N. D. KRAUT, N. KEBEDE, AND G. J. HOFFMAN

248th National Meeting of the American Chemical Society

San Francisco, CA

Aug. 2014

## Student Training

- 2019– **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

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## Teaching Experience

### INSTRUCTOR OF RECORD

#### Mathematical Methods for Chemical Physics

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.

School of Chemistry & Biochemistry | Georgia Tech

### 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-'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, semiempirical methods, molecular mechanics, transition-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 computational 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 assignments 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*

**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– **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– **Student Member: American Chemical Society**

## Skills

**Computational Chemistry Software** Psi4, Molpro, Q-CHEM, GAMESS, WebMO, Avogadro, PyMOL, VMD

**Programming** Python, Bash/Shell, LaTeX, C/C++

**Software Development** Git, GitHub, Open-Source Software Project Management

## References

### C. David Sherrill

PROFESSOR  
SCHOOL OF CHEMISTRY & BIOCHEMISTRY  
GEORGIA INSTITUTE OF TECHNOLOGY  
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### M.G. Finn

PROFESSOR AND CHAIR  
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901 ATLANTIC DR NW  
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MoSE 2201B  
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### Robert Dickson

VASSER WOOLLEY PROFESSOR  
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### Jesse McDaniel

ASSISTANT PROFESSOR  
SCHOOL OF CHEMISTRY & BIOCHEMISTRY  
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