

# Amanda Dumi

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## Education

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### University of Pittsburgh

PHD IN COMPUTATIONAL MODELING AND SIMULATION

GPA: 3.8

Pittsburgh, PA

Jun. 2017 - Exp. Sept. 2022

### Duquesne University

MASTER OF SCIENCE IN CHEMISTRY

GPA: 3.7

Pittsburgh, PA

Aug. 2015 - Dec. 2017

### Seton Hill University

BACHELOR OF SCIENCE IN CHEMISTRY

GPA: 3.8

Greensburg, PA

Aug. 2010 - May 2014

## Research Experience

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### Sandia National Laboratories

GRADUATE TECHNICAL INTERN

Albuquerque, NM

September. 2021 - PRESENT

- Working with **Dr. Luke Shulenburger** and **Dr. Raymond C. Clay** on characterizing multideterminant wave functions for periodic systems and Jastrow factor development

Pittsburgh, PA

GRADUATE RESEARCHER

Jul. 2017 - PRESENT

- Working with **Dr. Kenneth D. Jordan** on accurately describing non-valence correlation-bound anions using selected configuration interaction and quantum Monte Carlo methods
- Working with **Dr. Daniel S. Lambrecht** to identify a method for automated fragmentation of molecular species for computational approximations of large polymers

### Duquesne University

GRADUATE RESEARCHER

Pittsburgh, PA

Jul. 2015 - Jul-2017

- Working with Dr. Jeffrey D. Madura on improving the description of transport properties in materials using quantum Monte Carlo to benchmark density functional theory
- Working with Dr. Jeffrey D. Madura on describing the thermoelectric properties of pure and iodine-substituted  $\text{Bi}_2\text{Te}_3$

## Publications

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### The binding of atomic hydrogen on graphene from density functional theory and diffusion Monte Carlo calculations

AMANDA DUMI, SHIV UPADHYAY, LEONARDO BERNASCONI, HYEONDEOK SHIN, ANOUAR BENALI, KENNETH D. JORDAN

Journal of Chemical Physics, 2022; 156, 144702. DOI: 10.1063/5.0085982

### Q-GPU: A Recipe of Optimizations for Quantum Circuit Simulation Using GPUs

YILUN ZHAO, YUAN YAO, YANAN GUO, AMANDA DUMI, DEVIN M MULVEY, SHIV UPADHYAY, YOUTAO ZHANG, KENNETH D JORDAN, JUN

YANG, XULONG TANG

In Proceedings of the 28<sup>th</sup> IEEE International Symposium on High-Performance Computer Architecture, 2022 DOI: 10.1109/HPCA53966.2022.00059

### The Role of High-Order Electron Correlation Effects in a Model System for Non-valence Correlation-bound Anions

SHIV UPADHYAY, AMANDA DUMI, JAMES SHEE, KENNETH D. JORDAN

Journal of Chemical Physics, 2020, Dec 14; 153(22):224118. DOI: 10.1063/5.0030942

# Presentation

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## ORAL

- MOLECULAR FRAGMENT DETERMINATION WITH UNSUPERVISED MACHINE LEARNING TO RECOVER ELECTRONIC POLARIZABILITIES IN OLIGOMERIC SYSTEMS. 2022  
American Chemical Society, March Meeting
- CHEMICALLY INFORMED FRAGMENT CHOICES TO IMPROVE THE PROPERTY PREDICTION FOR POLYMER SYSTEMS 2021  
American Physical Society, March Meeting | Virtual
- THERMOELECTRIC PROPERTIES OF IODINE-SUBSTITUTED BISMUTH TELLURIDE USING WEIN2K 2016  
American Chemical Society National Meeting | San Diego, CA

## POSTER

- THE BINDING OF ATOMIC HYDROGEN ON GRAPHENE FROM DENSITY FUNCTIONAL THEORY AND DIFFUSION MONTE CARLO CALCULATIONS 2022  
Molecular Quantum Mechanics Conference | Blacksburg, VA
- IMPROVING QUANTUM CHEMISTRY WORKFLOWS WITH CCLIB: ENABLING EASIER POST-PROCESSING BY UNIVERSALLY REPRESENTING QUANTUM CHEMISTRY LOGFILES 2022  
Molecular Quantum Mechanics Conference | Blacksburg, VA
- TOWARDS TREATING THE NON-VALENCE CORRELATION-BOUND ANION OF TCNE WITH QUANTUM MONTE CARLO 2021  
Advanced Research Through Computing symposium | Pittsburgh PA
- PERFORMANCE OF AUTOMATIC FRAGMENTATION FOR PROPERTY PREDICTION 2020  
[recording link](#)  
Quantum 2020 | Pittsburgh PA
- CHEMICALLY INFORMED AUTOMATIC FRAGMENTATION 2020  
Finalist; [recording link](#)  
Pittsburgh Quantum Institute 2020 | Pittsburgh PA
- TOWARDS AN ACCURATE POTENTIAL ENERGY SURFACE OF  $\text{HCO}_2^-\cdot(\text{H}_2\text{O})$  USING CIPSI 2019  
Electronic Structure Workshop 2019 | Urbana-Champaign, IL  
QMCPack User Group Meeting 2019 | Oakridge, TN
- AUTOMATIC FRAGMENTATION FOR THE PREDICTION OF MOLECULAR PROPERTIES 2018  
Pittsburgh Quantum Institute 2019 Conference | Pittsburgh, PA
- TOWARDS AUTOMATIC FRAGMENTATION FOR ENERGY DECOMPOSITION ANALYSIS 2018  
Pittsburgh Quantum Institute Science Conference | Pittsburgh, PA
- TOWARDS REDUCING THE EFFECTS OF PSEUDOPOTENTIALS ON QUANTUM MONTE CARLO 2017  
Telluride School on Stochastic Methods in Electronic Structure | Telluride, CO
- CHARACTERIZING THE EFFECT OF PSEUDOPOTENTIALS ON QUANTUM MONTE CARLO CALCULATIONS 2017  
Pittsburgh Quantum Institute Conference | Pittsburgh, PA
- BENCHMARKING OF DENSITY FUNCTIONAL THEORY FUNCTIONALS WITH QUANTUM MONTE CARLO FOR AN ACCURATE DESCRIPTION OF THERMOELECTRIC MATERIALS 2017  
Pittsburgh Quantum Institute Conference | Pittsburgh, PA

# Professional Activities

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## Contributions to Open Source Software

2019-present

- cclib core developer
- Contributed to the following open source software packages: Avogadro2, PISCES, chemreps,iodata

## Journal Reviews

- Journal of Open Source Software 2020  
This journal adopts open peer reviews, the submissions I have reviewed are linked: 1, 2

## Quantum Monte Carlo Summer Workshop

Pittsburgh, PA

STUDENT INSTRUCTOR

2019

- Assisting students in understanding concepts and completing programming assignments on various quantum Monte Carlo methods
- Hosting and directing students and instructors visiting the area

## Statistical Mechanics Graduate Course

Pittsburgh, PA

STUDENT AID

2019

- Developing materials to create a graduate student assignment which introduces the conceptual foundations of the 1D and 2D Ising Model through Python exercises
- Grading and providing feedback to students on homework assignments

## Quantum Mechanics/Molecular Mechanics Study Group

Pittsburgh, PA

INSTRUCTOR

2018 - PRESENT

- Creating materials and teaching graduate students the theory and coding approaches to computational chemistry methods (hosted online)
- Planning and facilitating interdepartmental graduate student groups on advanced topics

## Citizen Science Lab

Pittsburgh, PA

INSTRUCTOR

2016 - PRESENT

- Guiding high school students to design experiments, characterize data, and present on improving microbial fuel cells created from local resources
- Developing materials to teach data collection, data visualization, and programming basics (hosted online)

## Undergraduate Mentor

Pittsburgh, PA

UNIVERSITY OF PITTSBURGH & DUQUESNE UNIVERSITY

2016 - 2017

- Teaching students to use computational resources, organize research, and theoretical approaches in chemistry
- Providing feedback on scientific communication for presentation and documents

## Phi Lambda Upsilon (Chemistry Honors Organization)

Pittsburgh, PA

MEMBER

Jan. 2015 - Dec. 2017

- Organizing an interdepartmental symposium
- Participating and organizing outreach events for middle school students

## Additional Volunteer Experience

- Free Ride bicycle collective; Pittsburgh, | 2022-present
- Poster Judge; Taylor Alderdice Highschool | 2020
- Poster Judge; Pennsylvania Junior Science Academy State Competition | 2016-2019
- National Chemistry Week Instructor; Carnegie Science Center | 2010-12, 2014
- Women in Science Day Guide; Seton Hill University | 2011-13
- Habitat for Humanity; Oak Ridge, TN | 2014
- PittCon Student Aide; Philadelphia, PA & Chicago, IL | 2013-14
- Young Chemist Carnival; Carnegie Mellon University | 2013

## Work Experience

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### Duquesne University

Pittsburgh, PA

TEACHING ASSISTANT

Jul. 2015 - May 2017

- Prepared lecture materials & quizzes for General Chemistry recitation
- Provided tutoring for group and individual needs

### Carnegie Science Center

Pittsburgh, PA

INTERN/EMPLOYEE

Jun 2013 - Sep 2014

- Presented shows teaching chemistry, physics, and biology to adults & children through engaging demonstrations
- Developed demonstrations, script, & staff safety measures for a new chemistry show

## Honors & Awards

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2021 **Advanced Research through Computing symposium Poster Award**  
2018 **Pittsburgh Quantum Institute Poster Award**  
2014 **Society of Analytical Chemists Award**  
2014 **Who's Who Among American Universities Award**  
2011 **CRC Press Chemical Achievement Award**  
2014 **The Sister Leon Bettwy Chemistry Award**  
2011 **Club of the Year Award; Chemistry Club**  
2010-14 **Dean's List**

*University of Pittsburgh*  
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*Seton Hill University*  
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