

Amanda Dumi

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Education

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

Jul. 2015 - Dec. 2017

Seton Hill University

BACHELOR OF SCIENCE IN CHEMISTRY

GPA: 3.8

Greensburg, PA

Aug. 2010 - May 2014

Research Experience

Sandia National Laboratories

GRADUATE TECHNICAL INTERN

Albuquerque, NM

September. 2021 - PRESENT

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

University of Pittsburgh

GRADUATE RESEARCHER

Pittsburgh, PA

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. Jeffry D. Madura on improving the description of transport properties in materials using quantum Monte Carlo to benchmark density functional theory
- Working with Dr. Jeffry D. Madura on describing the thermoelectric properties of pure and iodine-substituted Bi_2Te_3

Publications

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 28th IEEE International Symposium on High-Performance Computer Architecture, 2022

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

ORAL

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

POSTER

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

Professional Activities

Contributions to Open Source Software

2019-present

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

Journal Reviews

- Journal of Open Source Software
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)

University of Pittsburgh & Duquesne University

Pittsburgh, PA

UNDERGRADUATE MENTOR

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

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

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