Amanda **Dumi**

724.433.7825 | amandadumi@pitt.edu | amandadumi | @ae_dumi

Education

University of Pittsburgh — *Pittsburgh, PA*
PhD in Computational Modeling and Simulation — *Jun. 2017 - Exp. Sept. 2022*
GPA: 3.8

Duquesne University — *Pittsburgh, PA*
Master of Science in Chemistry — *Jul. 2015 - Dec. 2017*
GPA: 3.7

Seton Hill University — *Greensburg, PA*
Bachelor of Science in Chemistry — *Aug. 2010 - May 2014*
GPA: 3.8

Research Experience

Sandia National Laboratories — *Albuquerque, NM*
Graduate Technical Intern — *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 — *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 — *Pittsburgh, PA*
Graduate Researcher — *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

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 — *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)

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

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

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. *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

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 $HCO_2^-\cdot(H_2O)$ 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

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