# CAITLIN A. WHITTER

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## EDUCATION

**Purdue University**, College of Science
Ph.D. Student, *Computer Science*, GPA 3.6, Advisor: Professor Alex Pothen
West Lafayette, IN | 2018 – 2026 (expected)

**Purdue University**, College of Science
Master of Science, *Computer Science* | 2018-2024

**The George Washington University**, School of Engineering and Applied Science
Bachelor of Science, *Computer Science*
Washington, DC | 2014 - 2018
Honors: Clark Engineering Scholarship Program, University Honors Program, Dean's List,
Presidential Academic Scholarship, Southwest Neighborhood Assembly Scholarship

**Queen Mary University of London**, Study Abroad Program, Spring 2017

## RESEARCH INTERESTS

Caitlin explores research questions at the intersection of machine learning and computational science. Her Ph.D. research focuses on developing interpretable machine learning pipelines for accurately and efficiently predicting molecular and atomic properties from quantum-mechanical datasets.

## DOCTORAL FELLOWSHIPS

**Molecular Sciences Software Institute** Graduate Student Software Fellowship (2024-2025)
**D.E. Shaw Research** Doctoral and Postdoctoral Fellowship (2024)
**Department of Energy** Computational Science Graduate Fellowship [DOE CSGF] (2018 – 2022)
Practicum Location: Lawrence Berkeley National Laboratory
**National GEM Consortium** Graduate Fellowship (2018 – 2023)
Employer Sponsor: MIT Lincoln Laboratory

## SELECTED RESEARCH POSTIONS AND INTERNSHIPS

**Purdue University**
Department: Computer Science
*Ph.D. Student Researcher* | *Graduate Research Assistant* | West Lafayette, IN | Fall 2018 – Present

- Designed a physics-informed graph neural network for highly accurate prediction of molecular and atomic properties.
- Developed a scalable adaptive sampling algorithm that leads to greater neural network predictive performance compared to other subset selection algorithms, tested on several Image/NLP datasets and model architectures.
- Designing subset selection metrics to choose informative subsets from chemistry datasets to improve neural network performance and ascertain details about the underlying distribution of the datasets.

**Qualcomm |** Product and Test Engineering Team
*Summer Engineering Intern* | San Diego, CA | Summer 2024

- Developed a Python package for automating the identification of the type, location, and behavior of digital logic test failures in defective integrated circuits.
- Contributed to the development of a convolutional neural network classifier for failure debug, using PyTorch.

**Lawrence Berkeley National Laboratory (LBL)**
Division: Computational Research (Computing Science)
*DOE CSGF Summer Research Fellow* | Berkeley, CA and Remote Location | Summers 2019 and 2021

- Performed research on machine learning-based summarization algorithms for scientific datasets.
- Performed research on preconditioning techniques and graph kernels.

**MIT Lincoln Laboratory (MITLL)**
Division: Space Systems and Technology | Group: Advanced Sensors and Techniques
*Summer Research Intern* | Lexington, MA | Summer 2018
Developed an image reconstruction pipeline for generating high-resolution images of space objects under bandwidth-limited conditions.

**The George Washington University |** Department of Computer Science
PEMDAS | *Undergraduate Research Assistant* | Washington, DC | Fall 2017 – Spring 2018
Developed natural language processing algorithms to auto-generate conceptual math questions, plausible incorrect answers, and corresponding images for a mathematics education application.

**Qualcomm |** Qualcomm Cyber Security Solutions Division (Formerly: QGov)
*System Integration and Test Engineering Intern* | San Diego, CA | Summer 2017
Created a directed graph-based data visualization tool that takes in data from multiple sources throughout the division, finds unique relationships, and presents several visualizations of the data.

**The George Washington University |** Department of Computer Science
CAPITAL | *Undergraduate Research Assistant* | Washington, DC | Spring – Winter 2016
- Added user registration, editing, enrollment, and viewing pages to a reading comprehension education application that helps English-speaking adults gain literacy.
- Implemented a four-stage system in the back-end for course and exercise releases.

**U.S. Naval Research Laboratory |** Naval Research Enterprise Internship Program
*Summer Research Intern* | Washington, DC | Summer 2015
- Programmed an access point for humans to override the automated controls of a UAV simulation.
- Integrated Monte Carlo planner to allow humans to incorporate automated suggestions into their decision-making.

## PUBLICATIONS

- **Under Review:** Caitlin Whitter, Alex Pothen, and Aurora Clark. PIL-Net: Physics-Informed Graph Convolutional Network for Predicting Atomic Multipoles. *Digital Discovery*, 2025.
- **In Preparation for Submission:** Caitlin Whitter, Young In Kim, and Rajiv Khanna. FARS: A Flatness-aware Adaptive Random Sampling Algorithm for Subset Selection from Heterogeneous Data.
- Whitter, C.A., Alford, R., Aha, D.W., & Karneeb, J. (2015). Programming a human interaction access point for a virtual air combat simulation environment (Technical Note AIC-015-188). Washington, DC: Naval Research Laboratory, Navy Center for Applied Research on Artificial Intelligence.

## ACADEMIC SERVICE

International Joint Conference on Artificial Intelligence (IJCAI)
- Program Committee Member (2025)
- Reviewer (2024)

## CONFERENCES /WORKSHOPS

**Molecular Sciences Software Institute** | Software Fellow Bootcamp (Summer 2024)
- Presented my fellowship research project proposal to software scientists and other fellows.
- Participated in a hands-on one-week software best practices workshop.

**D.E. Shaw Research |** Doctoral and Postdoctoral Fellowship
New York, NY (Spring 2024)
- Gave research talk and presented research poster: PIL-Net: Physics-Informed Graph Convolutional Network for Predicting Atomic Multipoles

**ATPESC |** Argonne Training Program on Extreme-Scale Computing
St. Charles, IL (Summer 2023)
- Participated in an intensive two-week workshop on applying high performance computing to computational science and engineering applications.

**CMD-IT/ACM |** Richard Tapia Celebration of Diversity in Computing Conference
Washington, DC (Fall 2022) | Received full scholarship from Purdue CS Department.

**DOE Computational Science Graduate Fellowship** | Annual Program Review
Arlington, VA | Remote Location (Summer 2018-2022)
- Gave research talk: "Physics-Informed Prediction of Molecular Properties using a Graph Convolutional Network" (2022)
- Presented research poster: "Molecular Property Prediction with Graph Neural Networks" (2021)
- Presented research poster: "Preconditioning Techniques for the Marginalized Graph Kernel" (2019)

**Society for Industrial and Applied Mathematics |** Conference on Computational Science and Engineering (CSE21) | Remote Location (Spring 2021)
- Gave research talk: "Predicting Chemical Properties with Graph Neural Networks"

**Anita Borg Institute** | Grace Hopper Celebration of Women in Computing
Orlando, FL / Houston, TX (Fall 2017, 2016)
- Received full scholarships from the Anita Borg Institute and the Department of Computer Science at The George Washington University.

## TECHNICAL SKILLS

Python, Java, C, MATLAB, PyTorch, Deep Graph Library, RDKit, Linux, Git, MySQL, HTML/CSS, JavaScript

## INSTRUCTION

**Purdue University** | Graduate Teaching Assistant (Spring 2024)
Data Engineering in Python (CS 176)

**The George Washington University** | Undergraduate Teaching Assistant (2016-2018)

- Introduction to Software Development (CSCI 1111)
- Algorithms and Data Structures (CSCI 1112)
- Introduction to Software Development (CSCI 1111)

## RELEVANT PHD COURSEWORK

CS 580 | Algorithm Design, Analysis, and Implementation | A
CS 573 | Data Mining | A
CS 578 | Statistical Machine Learning | A-
CHM 579 | Computational Chemistry | A
STAT 511 | Statistical Methods | A
CS 525 | Parallel Computing | A

## SELECTED LEADERSHIP/MEMBERSHIPS

Purdue University:
**LEAP Alliance (Diversifying Leadership in the Professoriate)** | *PhD Fellow* (2022-)
**Computer Science Graduate Student Association** | *Webmaster* (2018-22), *Member* (2018-)
**Women in Science Programs** | Volunteered as computer science instructor for high school students (2019, 2023)
The George Washington University:
**Women in Computer Science** | *Co-President* (2017-18)
**National Society of Black Engineers** | *Treasurer* (2015-16)*, Freshman Representative* (2014-15)
**School of Engineering and Applied Science Student Peer Advisory Network** | *Mentor* (2016-18)
**Society of Women Engineers** | *SWENext Volunteer* (2016-18)
**Association for Computing Machinery** | *Member* (2015-18)