

Dilnoza Amirkulova (Permanent Resident)

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347-279-7323

University of Rochester
Department of Chemical Engineering
4008 Wegmans Hall
Rochester, NY, 14627

Highlights Combining computer science and chemical engineering in research
Extensive teaching and mentoring skills
Communicating in multiple languages

Education **Ph.D. Candidate, Chemical Engineering**, University of Rochester, Rochester NY, expected March, 2020
Adviser: Professor Andrew White
B.S., Biochemistry (*Cum Laude*), State University of New York (SUNY), Geneseo NY, 2014
Minor in Mathematics

Research Experience *Graduate Research Assistant, University of Rochester*, 2014–present
Adviser: Professor Andrew White

- Studied structure and dynamics of small molecules using simulations and experiments: peptides, RNA, proteins.
- Developed, maintained, and improved a Python package for simulations and enhanced sampling of molecules in GROMACS.
- Implemented HOOMD-TF, a tool to perform Machine Learning and Data manipulation in TensorFlow during HOOMD simulations.
- Implemented Experiment Directed Simulation for NMR and NOESY spectroscopy
- Mentored PhD, Master's and undergraduate students in the laboratory
- Created an educational web-based Molecular Dynamics simulator using JavaScript.

Graduate Research Intern, Zhejiang University, China, Summer 2019

Adviser: Professors Yi He and Andrew White

- Simulated a zwitterionic peptide E_6K_6 in HOOMD-TF
- Trained PhD students to use HOOMD-TF and HOOMD

Undergraduate Research Assistant, SUNY at Geneseo, 2012–2014

Adviser: Professor Eric Helms

- Organic synthesis expertise in synthesizing Atropic Acid
- Ran NMR and other experiments to characterize and to purify the synthesis products
- Isolated and purified Acetylenase gene in *Anaphalis margaritacea* plant
- Studied Acetylenase and Dehydrogenase gene expression of *Anaphalis margaritacea*

Teaching Experience *Teaching as Research Fellow, University of Rochester*, 2019
Professors Andrew White, April Luehmann, and Dr. Nickolas Hammond
Course: Numerical Methods and Statistics

Interim Lecturer, University of Rochester, 2018

Professor Andrew White

Course: Advanced Numerical Methods

Teaching Assistant, University of Rochester, 2015, 2017

Professor Andrew White

Course: Numerical Methods and Statistics

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Teaching Experience Cont.	<i>Teaching Assistant, University of Rochester</i> , 2016 Professor Wyatt Tenhaeff Course: Polymer Chemistry <i>Assistant Lab Instructor, SUNY at Geneseo</i> , 2013 Professor Kazushige Yokoyama Course: General Chemistry <i>Tutor, SUNY at Geneseo</i> , 2011-2014 Access Opportunity Program Courses: General Chemistry, Calculus, Biochemistry, Physical Chemistry, and Organic Chemistry.
Leadership Experience	<i>Graduate Student Association (GSA) Social Programmer University of Rochester</i> , 2019-present <i>GSA Grant Reviewer, University of Rochester</i> , 2016, 2018 <i>GSA Department Representative, University of Rochester</i> , 2017, 2018
Publications	Barrett R, Chakraborty M, Amirkulova DB , Gandhi HA, White AD (2019). Using GPU-Accelerated Tensor Operation Graphs in Molecular Simulation: HOOMD-Blue with TensorFlow. <i>Submitted</i> . Amirkulova DB , White AD (2019). Experiment Directed Ensemble Simulation of A β Peptide Fragment Consistent with NMR Experiments. <i>Submitted</i> . Amirkulova DB , White AD (2019). Recent Advances in Maximum Entropy Biasing Techniques for Molecular Dynamics. https://doi.org/10.1080/08927022.2019.1608988 MOLECULAR SIMULATION, 45. Amirkulova DB , White AD (2018). Combining Enhanced Sampling with Experiment Directed Simulation of the GYG peptide. <i>J. Theor. Comput. Chem.</i> (Special Issue), https://doi.org/10.1142/S0219633618400072 . 17(03).
Talks	Amirkulova DB , Free Energy Landscape with Experiment Directed Simulations and Enhanced Sampling, AICHE. Pittsburgh, PA, October, 2018. Amirkulova DB , Self-Assembly of Amyloid Peptide Fragments with Experiment Directed Simulations, AICHE. Pittsburgh, PA, November, 2018. Amirkulova DB , Breaking the Wall between Experiments and Simulations, Falling Walls Lab Competition. Rochester, NY, October, 2018. Amirkulova DB , Experiment Directed Simulations and Enhanced Sampling, Mid West Thermodynamics and Statistical Mechanics Conference. Pittsburgh, PA, June, 2018. Amirkulova DB , Lightning Talks, Frontiers in Materials Science for the 21st Century Symposium. Rochester, NY. May 25, 2017.
Posters	Amirkulova DB , Barrett R, Chakraborty M, Gandhi H, White AD. HOOMD-TF: Experiment Directed Simulation Application. Atlanta, GA. MLSE. June, 2019. Amirkulova DB , Chakraborty M, White AD. Bridging Nano and Macro Scale. Center for Emerging & Innovative Sciences. Rochester, NY. April, 2018. Amirkulova DB , Chakraborty M, White AD. ROC Sci-Tec Symposium. Rochester, NY. April, 2018. Amirkulova DB , White AD. Studying the structure and dynamics of A β ₂₁₋₃₀ with simulations and experiments. Minneapolis, MN. AICHE Annual Meeting, October, 2017. Amirkulova DB , White AD. Biasing Simulations with NMR results to study amyloid peptide. Frontiers in Materials Science for the 21st Century Symposium. Rochester, NY. May, 2017. Amirkulova DB , White AD. Matching Experiments with Simulations. Center for Integrated Research Computing's Annual Poster Session. Rochester, NY. May, 2017. Amirkulova DB , Chakraborty M, White AD. Implementing Experiment Directed Simulations. 252 nd ACS National Meeting. Philadelphia, PA. August, 2016.

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Skills	Python, JavaScript, R, bash, Molecular Dynamics, Coarse-Graining, Enhanced Sampling, Machine Learning, Design of Algorithms, TensorFlow, MDAnalysis, data analytics, Parallel Computing, git, LINUX, UNIX, GROMACS, LAMMPS, Gaussian, HOOMD-blue, Ovito, VOTCA, VMD, Plumed, Latex, Uzbek (native), Russian (native), Tajik (native), Spanish (intermediate), German (beginner)
Affiliations	Phi Beta Kappa National Honors Society, American Institute of Chemical Engineering, American Chemical Society, Society of Women Engineers, Beta Beta Beta National Biology Honors Society, Gamma Sigma Epsilon Chemistry Honors Society, Phi Eta Sigma National Honors Society
Awards	Zhejiang University Summer Scholars Program , Zhejiang University, China, 2019 Travel Grant for Women in Data Science workshop and MLSE , MLSE, Atlanta,GA, 2019 Teaching as Research Fellowship , CIRTLL, Rochester, 2019 Travel Grant for MDAnalysis Workshop & Hackathon , MDAnalysis, Evanston, 2018 Hopeman Honors Award , University of Rochester, Rochester, 2014-2017 Graduate Student Fellowship , University of Rochester, Rochester, 2014–present Mary Robinson-Slabey '64 Annual Scholarship , SUNY, Geneseo, 2011–2014 Geneseo Foundation Research Fellowship , SUNY, Geneseo, 2013 Geneseo Foundation Scholarship , SUNY, Geneseo, 2011–2014 Dean's List , SUNY, Geneseo, 2010–2014 International Students Scholarship , SUNY, Geneseo, 2010–2014