

Dilnoza Amirkulova (Permanent Resident)

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University of Rochester
Department of Chemical Engineering
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Highlights	Combining chemistry, biology, and computer science in research Extensive teaching and mentoring skills Communicating in multiple languages
Education	Ph.D. Candidate, Chemical Engineering , University of Rochester, Rochester NY, March, 2020 Adviser: Professor Andrew White B.S., Biochemistry (<i>Cum Laude</i>), State University of New York (SUNY), Geneseo NY, 2014 Minor in Mathematics
Research Experience	<i>Graduate Research Assistant, University of Rochester</i> , 2014–present Adviser: Professor Andrew White

- Studied structure and dynamics of peptides using simulations and experiments
- Developed, maintained, and improved a python package, [Peptidesim](#), for automating simulations, enhanced sampling and biasing of peptides and proteins in GROMACS
- Wrote python code for biasing in [HOOMD-TF](#), a tool to perform Machine Learning and data analysis in TensorFlow during HOOMD simulations
- Improved Molecular Dynamics simulation by adding NMR and NOESY spectroscopy
- Mentored PhD, Master’s and undergraduate students in the laboratory
- Created an educational web-based Molecular Dynamics simulator, [JSMD](#), 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, 2012–2014

Adviser: Professor Eric Helms

- Organic synthesis, purification, and characterization expertise in atropic acid synthesis
- Isolated and purified Acetylenase gene in *Anaphalis margaritacea* plant
- Studied Acetylenase and Dehydrogenase gene expression of *Anaphalis margaritacea*

Skills	Python, JavaScript, R, bash, html, git, LINUX, UNIX, Molecular Dynamics, Coarse-Graining, Enhanced Sampling, Machine Learning, Design of Algorithms, TensorFlow, MDanalysis, data analytics, Parallel Computing, GROMACS, LAMMPS, Gaussian, HOOMD-blue, Ovito, VOTCA, VMD, Plumed, Latex, NMR, gel electrophoresis, gene isolation, column chromatography, Uzbek (native), Russian (native), Tajik (native), Spanish (intermediate), German (beginner)
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Leadership Experience	<i>Graduate Student Association (GSA) Social Programming Officer, University of Rochester</i> , 2019 <i>GSA Grant Reviewer, University of Rochester</i> , 2016, 2018 <i>GSA Department Representative, University of Rochester</i> , 2017, 2018 <i>Muslim Student Association Secretary, SUNY</i> , 2013, 2014
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- Publications** **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. *J. Theor. Comput. Chem.* (Special Issue), <https://doi.org/10.1142/S0219633618400072>. 17(03).
- Under Review** Barrett R, Chakraborty M, **Amirkulova DB**, Gandhi HA, White AD (2019). Using GPU-Accelerated Tensor Operation Graphs in Molecular Simulation: HOOMD-Blue with TensorFlow, <https://doi.org/10.26434/chemrxiv.8019527.v3> *Submitted*
- Amirkulova DB**, White AD (2019). Experiment Directed Ensemble Simulation of A β Peptide Fragment Consistent with NMR Experiments. *Submitted*
- In prep.** **Amirkulova DB**, White AD (2019). EK-based Zwitterionic Peptide Self-Assembly and Phase Diagrams
- Amirkulova DB**, Gandhi HA, White AD (2019). Modeling of A β 42 intramolecular interactions with Experimental Observables
- Teaching** *Teaching as Research Fellow, University of Rochester*, 2019
Center for the Integration of Research, Teaching and Learning, **CIRTL**
Interim Lecturer, University of Rochester, 2018
Course: Advanced Numerical Methods
Teaching Assistant University of Rochester, 2015, 2017
Course: Numerical Methods and Statistics
Teaching Assistant, University of Rochester, 2016
Course: Polymer Chemistry
Assistant Lab Instructor, SUNY at Geneseo, 2013
Course: General Chemistry
Tutor, SUNY at Geneseo, 2011-2014
Courses: General Chemistry, Calculus, Biochemistry, Physical Chemistry, and Organic Chemistry
- 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, and 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, Atlanta, GA, 2019
Teaching as Research Fellowship, CIRTL, 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
- Talks** **Amirkulova DB**, Molecular Dynamics Simulations of Zwitterionic Peptide Self-Assembly, AICHE. Orlando, FL, November, 2019
Amirkulova DB, Exploration of Interresidual Contacts in Combined Coarse Graining and Experiment Directed Simulations of A β 42, AICHE. Orlando, FL, November, 2019
Amirkulova DB, Free Energy Landscape with Experiment Directed Simulations and Enhanced Sampling, AICHE. Pittsburgh, PA, October, 2018

Talks

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, Chakraborty M, White AD. The Use of Experiment Directed Simulations to Improve the Accuracy of Simulations. Orlando, FL. AICHE. November, 2019

Amirkulova DB, Interactions of Amyloid Peptide Self-assembly, ROC Sci-Tech Symposium, Rochester, NY, October, 2019

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 $A\beta_{21-30}$ 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. 252nd ACS National Meeting. Philadelphia, PA. August, 2016