

**Dilnoza Amirkulova (Permanent Resident)**

damirkul@ur.rochester.edu  
dilnoza92@gmail.com

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

**Dilnoza Amirkulova (Permanent Resident)**

damirkul@ur.rochester.edu  
dilnoza92@gmail.com

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

---

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

**Dilnoza Amirkulova (Permanent Resident)**

damirkul@ur.rochester.edu

dilnoza92@gmail.com

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

---

|                     |   |
|---------------------|---|
| <b>Skills</b>       | 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)   |
| <b>Affiliations</b> | 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  |
| <b>Awards</b>       | <b>Zhejiang University Summer Scholars Program</b> , Zhejiang University, China, 2019<br><b>Travel Grant for Women in Data Science workshop and MLSE</b> , MLSE, Atlanta,GA, 2019<br><b>Teaching as Research Fellowship</b> , CIRTl, Rochester, 2019<br><b>Travel Grant for MDAnalysis Workshop &amp; Hackathon</b> , MDAnalysis, Evanston, 2018<br><b>Hopeman Honors Award</b> , University of Rochester, Rochester, 2014-2017<br><b>Graduate Student Fellowship</b> , University of Rochester, Rochester, 2014–present<br><b>Mary Robinson-Slabey '64 Annual Scholarship</b> , SUNY, Geneseo, 2011–2014<br><b>Geneseo Foundation Research Fellowship</b> , SUNY, Geneseo, 2013<br><b>Geneseo Foundation Scholarship</b> , SUNY, Geneseo, 2011–2014<br><b>Dean's List</b> , SUNY, Geneseo, 2010–2014<br><b>International Students Scholarship</b> , SUNY, Geneseo, 2010–2014 |