Geyao Gu

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EDUCATION

Northwestern University, Evanston, IL (Anticipated) June 2025
PhD, Physical Chemistry GPA: 3.90/4.00

University of Science and Technology of China, Hefei, China June 2019
BS, Chemical Physics GPA: 3.73/4.30

SKILLS

Programming Language	Python, R, C, C++, Jupyter, Mathematica, Bash
Softwares	GROMACS, Gaussian
Domain Knowledge	Molecular Dynamics, Thermodynamics, Statistical Mechanics, Machine Learning
Tools & Libraries	Git, Numba, Pandas, Scipy, Numpy, Scikit-learn, Pytorch, joblib

RESEARCH EXPERIENCE

Northwestern University, Evanston, IL
Graduate Research Assistant, Gingrich Group, Department of Chemistry September 2019 - Present

- Discovered the conditions under which mechanical coupling enhances the speed of synthetic chemically-fueled molecular motors by over 50%, using nonequilibrium molecular dynamics (MD) simulations and a jump-diffusion model.
- Found reduced directional bias through mechanical coupling by impairing chemical gating in synthetic motors, a characteristic shared with biological motors.
- Rationalized the role of the power stroke in molecular motors by coarse-graining MD simulation data into a Markov State Model and identifying key transition pathways.
- Identified a mechanism to reverse the directionality of molecular motors via steric hindrance, revealing from MD simulations.
- Mentored two undergraduate students on simulating molecular motors and molecular pumps, contributing to research works currently in preparation.

University of Wisconsin, Madison, WI
Research Assistant, Van Lehn Group, Department of Chemical and Biological Engineering July 2017 - August 2017

- Performed free energy calculations for solvation of hydronium ion in the mixed water-cosolvent environments to analyze hydrolysis and elimination reactions of hydrophilic (-OH) substrates with Brønsted-acid catalysts in the mixed water-cosolvent environments.
- Calculated dielectric constant and hydrogen bond statistics to interpret the results in free energy calculations.

University of Science and Technology of China, Hefei, China
Research Assistant, Hefei National Laboratory for Physical Sciences at the Microscale September 2017 - June 2019

- Calculated electronic structures in ground and excited states with both QM/MM and QM(PCM) methods in varied solvents to study aggregation emission of chromophore amphiphiles in solution.
- Probed the solvent effects on the conformation of the target molecules using MD.

PUBLICATIONS

1. **Gu, Geyao**, Drew Alvarez, John Strahan, Alex Albaugh, Emanuele Penocchio, and Todd R Gingrich. It takes two to make a thing go right: Boosting current in coupled motors. *Manuscript complete; in submission preparation.*, 2025
2. Emanuele Penocchio, **Gu, Geyao**, Alex Albaugh, and Todd R. Gingrich. Power strokes in molecular motors: Predictive, irrelevant, or somewhere in between? *Journal of the American Chemical Society*, 147(1):1063–1073, 2025
3. Alex Albaugh, **Geyao Gu**, and Todd R Gingrich. Sterically driven current reversal in a molecular motor model. *Proceedings of the National Academy of Sciences*, 120(33), 2023
4. Alex Albaugh, Rueih-Sheng Fu, **Geyao Gu**, and Todd R Gingrich. Limits on the precision of catenane molecular motors: Insights from thermodynamics and molecular dynamics simulations. *Journal of Chemical Theory and Computation*, 2023

PRESENTATIONS

1. Optimizing a Chemically-Fueled Molecular Motor, *APS March Meeting*, 2022.
2. Designing a chemically-fueled molecular motor via simulations, *Berkeley Statistical Mechanics Meeting*, 2023.

TEACHING EXPERIENCE

Northwestern University, Evanston, IL
Lecture Teaching Assistant, Quantum Chemistry I (Fall 2022)

- Communicated with students of diverse backgrounds by quickly identifying common challenges and individual needs during office hours, providing detailed guidance to those with weaker foundations while fostering collaborative group discussions among others.

Northwestern University, Evanston, IL
Lab Teaching Assistant, Advanced General Inorganic Chemistry Laboratory I (Fall 2019), *Advanced General Inorganic Chemistry Laboratory II* (Winter 2020), *Introductory Instrumental Analysis* (Spring 2020), *General Chemistry Laboratory II* (Summer 2020).

- Prepared and delivered prelab lectures that effectively engaged small groups by explaining lab principles at a high level and sparking interest in the experiment.
- Recognized students' diverse needs and provided personalized support by motivating independent students to think deeper and broader while patiently guiding those requiring more attention, ultimately leading one student to join the research group.

LEADERSHIP AND SERVICE

Northwestern University, Evanston, IL
Committee Member of TCSS (Theoretical Chemistry Seminar Series) August 2022 - Present

- Nominate speakers from the Chicago area and coordinate theoretical chemistry talks at Northwestern University.

Northwestern University, Evanston, IL
Chair of Faith-Hope-Love Christian Fellowship September 2021 - December 2022

- Organized regular Bible studies and special events.