

Kristina Trifonova

Curriculum Vitae

✉ ktrifonova@uchicago.edu
 🌐 k-trifonova.github.io

Education

- 2023–Present **Ph.D. in Theoretical Physical Chemistry**, *University of Chicago*, Chicago, IL
 Co-advised by Prof. Suri Vaikuntanathan and Arvind Murugan
- 2023–2024 **M.S. in Chemistry**, *University of Chicago*, Chicago, IL
- 2019–2023 **B.S. in Engineering Science & Chemistry**, *Emory University*, Atlanta, GA
 ○ **Honors thesis:** *Optimizing a Bifurcating [NiFe]-Hydrogenase System for Light-Driven Hydrogen Production*, supervised by Prof. Bryan Dyer, highest honors
- 2025 **The Beg Rohu Summer School of Physics**, *École Normale Supérieure*, Saint-Pierre-Quiberon, France
 Topic: Learning with Machines, Physics, and Minds

Experience

Research

- 2023–Present **Graduate Researcher**, *Vaikuntanathan & Murugan Groups*, University of Chicago
 Working with professors Arvind Murugan and Suri Vaikuntanathan to explore the inherent information processing and computational abilities of biophysical processes, like phase separation and reaction networks, using statistical mechanics and machine learning theory.
- Summer 2022 **Summer Researcher**, *Olmsted Group*, Georgetown University
 Worked with professor Peter Olmsted as part of NSF REU in Materials Physics, developing and analyzing molecular dynamics simulations to study the unusual properties of water confined to the stratum corneum lipid matrix of the skin.
- 2021–2023 **Undergraduate Researcher**, *Dyer Group*, Emory University
 Worked under the supervision of professor Bryan Dyer, spectroscopically investigating the mechanism of electron bifurcation by developing a model system for light-driven hydrogen production with CdSe quantum dots and [NiFe]-hydrogenase enzymes.

Teaching

- 2023–2024 **Teaching Assistant**, *CHEM 111-113: General Chemistry*, University of Chicago
 ○ Led weekly recitation, ran labs, held office hours, and graded lab reports and exams
 ○ Received 23-24 Physical Sciences Division Teaching Prize, based on student nominations
- Aug 2024 **Math Bootcamp Instructor**, *Multivariable Calculus*, University of Chicago
 ○ Developed a physical chemistry-focused lecture and accompanying problem set to help incoming graduate students refresh their math skills
- Spring 2025 **Grader**, *PHYS 491: Biological Physics*, University of Chicago
 ○ Wrote solutions and graded problem sets for graduate Biological Physics.

Publications and Manuscripts

- [1] **K. Trifonova***, L.H. Delgado-Granados*, L.M. Sager-Smith* and D.A. Mazziotti. Machine learning of two-electron reduced density matrices for many-body problems. *Journal of Physical Chemistry Letters*, 2025.

*: These authors contributed equally

Presentations

Contributed Talks (2)

April 2025 **In situ trainable computation in many-to-many molecular networks***, Foundations of Nanoscience Conference

Jan 2025 **Trainable computation in many-to-many molecular networks**, Gordon Research Conference on Stochastic Physics in Biology

*: Talk prize

Posters (6)

June 2025 **In situ trainable computation in many-to-many molecular networks**, Beg Rohu Summer School of Physics

Jan 2025 **Trainable computation in many-to-many molecular networks**, Gordon Research Conference on Stochastic Physics in Biology

Jan 2025 **Trainable computation in many-to-many molecular networks**, NITMB Workshop on Biological Systems that Learn

Nov 2024 **Computational expressivity and training of chemical reaction networks**, UChicago Center for Living Systems Symposium

June 2024 **Learning through non-equilibrium dynamics in molecular systems**, UChicago Physics of Evolution Symposium

July 2022 **Investigating confined water in the stratum corneum lipid matrix**, Georgetown Physics Summer Research Symposium

Fellowships, Awards, and Scholarships

2025 **FNANO Talk Award**, ISNSCE

2024 **Olshansky Graduate Travel Award**, University of Chicago

2024 **Physical Sciences Division Teaching Prize**, University of Chicago

2023 **McCormick Fellowship**, University of Chicago

2023-2028 **National Science Foundation Graduate Research Fellowship**

2023 **Shepard Scholarship**, Emory University

2022-2023 **William Jones Memorial Scholarship**, Emory University

2021 **Excellence in Undergraduate Support Award**, Emory University

2019-2023 **National Merit Scholar**, National Merit Foundation

2019 **Regeneron Science Talent Search Scholar**, Society for Science

Technical Skills

Technical:

- scientific computing, molecular dynamics simulations, convex optimization, autodiff, energy-based machine learning, contrastive learning, Monte Carlo, rare event simulation

Programming:

- Python (Numpy, Scipy, JAX, Tensorflow, Matplotlib), Java, Matlab, Mathematica, Maple, Git, Bash/shell, L^AT_EX

Software:

- GROMACS, PyMOL, VMD

Service

Conference Roles

- Jan 2025 **Discussion Leader**, *NITMB Workshop on Biological Systems that Learn*, "Function: What is it and how can we tell?"

Department Leadership Roles (Elected)

- 2024-2025 **Women+ in Chemistry Board Member**, *University of Chicago*

- Organized outreach events for gender minorities in the physical sciences, including career talks, book clubs, a grad school application coffee chat, and recruitment brunches
- As social presence coordinator, managed WiC+ website and advertised upcoming events

- 2024-2025 **First Year Journal Club Organizer**, *University of Chicago*

- Organized weekly journal club by and for first-year chemistry graduate students

- 2022-2023 **Chemistry Undergraduate Representative**, *Emory University*

- Member of Undergraduate Faculty Committee, advocated to reform advising guidelines and improve undergraduate research access and conducted departmental climate surveys
- Helped organize first-ever departmental town hall and get student representatives on all faculty committees

Outreach

- 2023-2024 **South Side Science Festival**, *University of Chicago*

- Member of DEI and Logistics planning committees, attended weekly meetings to organize event details for >4500 attendees
- Led interactive chemistry and physics demos for families

- 2023-2024 **Physics with a Bang**, *University of Chicago*

- Presented physics demos to students from local south side Chicago schools

- 2023-2024 **Mentor Match Engine**, *Illinois Science and Technology Coalition*

- Virtually mentored local high school students doing a year-long engineering project, from conception of the idea to building the final product

- October 2023 **Chemistry Alumni PhD Panel**, *Emory University*

- Organized and led panel aimed at undergrads interested in chemistry PhD programs
- Created online compilation of graduate school application resources that was shared with all Emory chemistry majors