# Kristina Trifonova

# Curriculum Vitae

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## Education

2023-Present **Ph.D. in Theoretical Physical Chemistry**, *University of Chicago*, Chicago, IL Co-advised by Prof. Arvind Murugan and Suri Vaikuntanathan

June 2025 **The Beg Rohu Summer School of Physics**, *École Normale Supérieure*, Saint-Pierre-Quiberon, France

O Topic: Learning with Machines, Physics, and Minds

2023-2024 M.S. in Chemistry, University of Chicago, Chicago, IL

2019–2023 B.S. in Engineering Science & Chemistry, Emory University, Atlanta, GA

O Honors thesis: Optimizing a Bifurcating [NiFe]-Hydrogenase System for Light-Driven Hydrogen Production, supervised by Prof. Bryan Dyer, highest honors

# Experience

#### Research

2023-Present **Graduate Researcher**, *Vaikuntanathan & Murugan Groups*, University of Chicago Working with professors Arvind Murugan and Suri Vaikuntanthan 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**

In Progress College Teaching Certificate, University of Chicago

 Completed pedagogical training program covering class design, instructional strategies, and practical teaching experience

2024-2025 Math Bootcamp Lead Organizer & Session Leader, University of Chicago

- Led pedagogical design and implementation of 2-week math preparation program for incoming chemistry grad students
- Managed end-to-end operations: TA coordination, funding acquisition and management, curriculum development, materials creation, and logistics
- Developed & taught multi-variable calculus sessions emphasizing group problem solving

Spring 2025 Grader, PHYS 491: Biological Physics, University of Chicago

O Wrote solutions and graded problem sets for graduate Biological Physics.

- 2023-2024 **Teaching Assistant**, CHEM 111-113: General Chemistry, University of Chicago
  - O Led weekly recitation, ran labs, held office hours, and graded lab reports and exams
  - O Received 23-24 Physical Sciences Division Teaching Prize, based on student nominations

# 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 (3)

- October 2025 In situ trainable computation in many-to-many molecular networks, HHMI Janelia Junior Scientist Workshop on Theoretical Biophysics
  - 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 (7)

- October 2025 In situ trainable computation in many-to-many molecular networks, HHMI Janelia Junior Scientist Workshop on Theoretical Biophysics
  - 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:

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

#### **Programming:**

O Python (Numpy, Scipy, JAX, Tensorflow, Matplotlib), Java, Matlab, Mathematica, Maple, Git, Bash/shell, LATEX

#### 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)

- 2024-2026 Women+ in Chemistry President, University of Chicago
  - Organized professional development, networking, community outreach, and social events events targeting underrepresented groups in the physical sciences
  - As president, oversaw planning of monthly events & facilitated engagement with other groups on campus and in Chicago
  - O As media coordinator, managed WiC+ website & advertised 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* 
  - $\circ$  Member of DEI and Logistics planning committees, attended weekly meetings to organize event details for >4500 attendees
  - O Led interactive chemistry and physics demos for families
- 2023-2024 Physics with a Bang, University of Chicago
  - O Presented physics demos to students from local south side Chicago schools

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

O 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
- $\,\circ\,$  Created online compilation of graduate school application resources that was shared with all Emory chemistry majors