Spencer Guo

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SUMMARY

- Biomolecular simulation and sampling expert with 6+ years of experience in molecular modeling
- Interdisciplinary collaborator with broad knowledge in structural and machine learning methods
- Scientific communicator and author of peer-reviewed publications in *Nature* and *PNAS*

EDUCATION

Ph.D. Chemistry, **The University of Chicago** 9/2020 – 6/2025 (expected)
Supervisors: Profs. Aaron Dinner and Benoît Roux
Thesis: Long-timescale kinetics and mechanisms of protein conformational change
Research interests: molecular dynamics simulations, protein kinetics, membrane proteins, machine-learning methods for statistical mechanics, integration of experimental biophysics data (cryo-EM, NMR, electrophysiology)

M.S. Chemistry, **The University of Chicago** 9/2020 – 9/2021

B.S. Biological Chemistry, **Stanford University**, *Minor in Computer Science* 9/2016 – 6/2020

RESEARCH + WORK EXPERIENCE

The University of Chicago Graduate Research Assistant
Department of Chemistry 9/2020 – present
– Applied dynamical analysis and enhanced sampling to elucidate membrane protein mechanisms
– Benchmarked a non-Markovian algorithm for computing kinetic statistics with short trajectories
– Developed an method leveraging pretrained GNNs to automatically featurize molecular structures
– Collaborated closely with experimentalists to integrate NMR and HDX data
– Wrote a successful grant application to obtain Anton supercomputer time for simulations

Stanford University Undergraduate Research Assistant
Department of Chemistry, Markland Lab 9/2018 – 6/2020
– Simulated IR spectra of liquid water using *ab initio* molecular dynamics
– Adapted a neural network method to calculate molecular dipoles

Schrödinger Python Development Intern
New York, NY 6/2019 – 9/2019
– Developed tool to identify critical residue/ligand interactions for drug development
– Extended multiple sequence viewer (MSV) to analyze similarity at binding sites

Genentech Protein Engineering Intern
South San Francisco, CA 6/2018 – 9/2018
– Synthesized novel peptide library for PROTAC optimization using rational macrocycle design
– Analyzed instrumental purity and spectral data (LC-MS, HPLC, NMR)

SERVICE EXPERIENCE

Science One-Pager Initiative
Illinois Science Policy Consortium 3/2024 – present
– Authored a one-page policy brief about therapeutic use of psychedelics for mental health disorders
– Summarize and synthesize scientific studies to support evidence-based policy in Illinois legislature

Modern Materials and Technology Volunteer
The University of Chicago 9/2021 – present

– Teach a weekly colloquium to ∼15 high school students in Chicago
– Create lesson plans demonstrating applications of chemistry and physics to modern technology

Department of Chemistry Director of Graduate Student Initiatives
The University of Chicago 7/2022 – 6/2023
– Served as liaison between graduate students and faculty to increase open communication
– Developed policies to alleviate student concerns and help their transition to graduate school
– Designed policies at cross-department weekly meetings and organize feedback from students

SKILLS

Technical	structural modeling, molecular dynamics simulations, enhanced sampling techniques, graph neural networks, Monte Carlo methods
Programming	(*experienced*) Python (NumPy/SciPy), jax, PyTorch, bash, git, LaTeX (*familiar*) C/C++, Matlab
Software	(*experienced*) Amber, OpenMM, VMD, MDAnalysis, Alphafold (*familiar*) GROMACS, BioPython, PyMOL, CP2K, DFTB+

PUBLICATIONS + PREPRINTS

* Denotes equal contribution.

1. K. Jeong, S. Guo, S. Allaw, & A. R. Dinner. Analysis of the dynamics of a complex, multipathway reaction: Insulin dimer dissociation. *J. Phys. Chem. B*, ASAP (2024).
2. N. Zhang*, D. Sood*, S. Guo*, N. Chen, *et al*. Temperature-Dependent Fold-Switching Mechanism of the Circadian Clock Protein KaiB. *Proc. Natl Acad. Sci. USA*, **121**, e2412327121 (2024).
3. Z. Pengmei, C. Lorpaiboon, S. Guo, J. Weare, & A. R. Dinner. geom2vec: pretrained GNNs as geometric featurizers for conformational dynamics. arXiv:2409.19838 (2024).
4. S. Guo, R. Shen, B. Roux, & A. R. Dinner. Dynamics of activation in the voltage-sensing domain of *Ciona intestinalis* phosphatase Ci-VSP. *Nat. Commun.* **15**, 1408 (2024).
5. C. Lorpaiboon, S. Guo, J. Strahan, J. Weare, & A. R. Dinner. Accurate estimates of dynamical statistics using memory. *J. Chem. Phys.* **160**, 084108 (2024).
6. J. Strahan, S. Guo, A. R. Dinner, & J. Weare. Inexact iterative numerical linear algebra for neural network-based spectral estimation and rare-event prediction. *J. Chem. Phys.* **159**, 014110 (2023).

PRESENTATIONS

Talk at **Center for Learning Systems Cell State Transitions Workshop**, *Chicago, IL* 5/2024
– Learning dynamical statistics from short-trajectory data
Poster at **IMSI "Learning Collective Variables and Coarse Grained Models" Workshop** 2/2024
– Inexact subspace iteration for neural network-based rare-event prediction
Invited lecture at **Associated International Laboratory (CNRS/UIUC)**, *Hauteluce, France* 1/2024
– Complex kinetics and mechanism of voltage activation in the voltage-sensing domain of Ci-VSP
Poster at **AI & Science Summer School 2023**, *Chicago, IL* 7/2023
– Inexact iterative numerical linear algebra for neural network-based spectral estimation and rare-event prediction
Poster at **Biophysical Society Annual Meeting**, *San Francisco, CA* 2/2022
– Dynamical analysis of voltage-dependent activation in Ci-VSP

AWARDS + GRANTS

St. Jude National Graduate Student Symposium, *St. Jude Children's Hospital* 2024
Anton 2 Biomolecular Simulation Grant, *Pittsburgh Supercomputing Center* 2021
NSF Graduate Research Fellowship, *National Science Foundation* 2020
Eckhardt Fellowship, *Physical Sciences Division, The University of Chicago* 2020

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