Hannah K. Wayment-Steele

wayment@brandeis.edu | www.hwaymentsteele.github.io

Education

Ph.D., Chemistry, Stanford University	2016 – 2021
Advisors: Rhiju Das, Vijay Pande	
M.Phil., Chemistry, Cambridge University	2015 – 2016
Advisor: Daan Frenkel	
B.A., Chemistry and Mathematics double major, Music minor, Pomona College	2011 – 2015

Honors and Awards

Jane Coffin Childs Postdoctoral Fellowship	2022
Award for Outstanding Graduate Research, *ACS PHYS division & J. Chem. Phys.*	2021
Chemical Computing Group Excellence Award, *ACS COMP division*	2021
Joseph R. McMicking Award, *Stanford Chemistry Department*	2021
NSF Graduate Research Fellowship	2016
Churchill Scholarship, *Sir Winston Churchill Foundation of the USA*	2015
John Stauffer Prize for Academic Merit in the Sciences*, *Pomona College*	2015
Beckman Scholar	2014
Goldwater Scholar	2014

*Awarded to one STEM graduate annually who exhibits the highest academic promise

Research

Postdoctoral Fellow, Brandeis University   2022 – present
   Advisor: Dorothee Kern
- Developed deep-learning-based approaches to predict multiple conformational states in proteins
- Created benchmarks of nuclear magnetic resonance (NMR) measurements of dynamics in proteins and integrated with state-of-the-art deep-learning approaches, including AlphaFold2 and language models
- Advised students in projects on protein language model interpretability

Visiting Faculty Researcher, Google Brain   Oct. 2022 – Apr. 2023
   Host: Lucy Colwell
- Consulted on projects using deep learning in structural biology and biotechnology

Postdoctoral Fellow, Wyss Institute, Harvard Medical School   2021 – 2022
   Advisor: William Shih
- Developed novel assays for ultra-sensitive biomolecule detection

Graduate research, Stanford University   2016 – 2021
- Developed improved algorithms for RNA thermodynamic prediction using statistical mechanics to link high-throughput experiment and machine learning
- Created biophysical models for RNA degradation, applied methods to design experimentally validated model mRNA therapeutics with improved shelf lives
- Linked dynamical systems theory and unsupervised machine learning frameworks to create improved analysis tools for molecular dynamics simulations of proteins

Graduate research, Cambridge University   2015 – 2016
- Improved understanding of DNA nanomaterial nucleation and assembly via molecular modelling

Peer-Reviewed Publications (*Equal contributions)

Ke, Y., Sharma, E., <u>Wayment-Steele, H. K.,</u> Becker, W. R., Ho, A., Marklund, E., Greenleaf, W. J. "High throughput DNA melt measurements enable improved models of DNA folding thermodynamics". (2024) *bioRxiv* 2024.01.08.574731.

Choe, C.A., Andreasson, J.O.L., Melaine, F., Kladwang, W., Wu, M. J., Portela, F., Wellington-Oguri, R., Nicol, J. J., <u>Wayment-Steele, H.K.,</u> Gotrik, M., Eterna Participants, Khatri, P., Greenleaf, W. J., Das, R. "Compact RNA sensors for increasingly complex functions of multiple inputs." (2024) *bioRxiv* 2024.01.04.572289.

<u>Wayment-Steele, H.K.*,</u> Ojoawo, A.*, Otten, R., Apitz, J.M., Pitsawong, W., Ovchinnikov, S., Colwell, L.J., Kern, D. "Predicting multiple conformations via sequence clustering and AlphaFold2". (2023) *Nature.*

<u>Wayment-Steele, H. K.*,</u> Kladwang, W.*, Watkins, A. M.*, Kim, D. S.*, Tunguz, B.*, ... Das, R. (2022) Deep learning models for predicting RNA degradation via dual crowdsourcing. *Nature Machine Intelligence* (4) 1174-84.

<u>Wayment-Steele, H.K.,</u> Kladwang, W., Strom, A. I., Becka, A., Lee, J., Treuille, A., Eterna Participants, Das, R. (2022). RNA secondary structure packages evaluated and improved by high-throughput experiments. *Nature Methods* (19) 1234-42.

Leppek, K.*, Byeon, G.W.*, Kladwang, W.*, <u>Wayment-Steele, H. K.*,</u> Kerr, C. H.*, ... Barna, M., Das, R. (2022) Combinatorial optimization of mRNA structure, stability, and translation for RNA-based therapeutics. *Nature Communications* (13) 1536*.*

Andreasson, J. O., Gotrik, M. R., Wu, M. J., <u>Wayment-Steele, H. K.,</u> Kladwang, W., Portela, F., Wellington-Oguri, R., Eterna Participants, Das, R., Greenleaf, W. J. (2022). Crowdsourced RNA design discovers diverse, reversible, efficient, self-contained molecular sensors. *Proceedings of the National Academy of Sciences* (119) 18.

<u>Wayment-Steele, H.K.,</u> Kim, D.S., Choe, C.A., Nicol, J.J., Wellington-Oguri, R., Sperberg, R.A.P., Huang, P., Eterna Participants, Das, R. (2021). Theoretical basis for stabilizing messenger RNA through secondary structure design. *Nucleic Acids Research*, 48(18), 10604-10617.

Kostrz, D., <u>Wayment-Steele, H. K.,</u> Wang, J. L., Follenfant, M., Pande, V. S., Strick, T. R., Gosse, C. (2019). A modular DNA scaffold to study protein–protein interactions at single-molecule resolution. *Nature Nanotechnology*, 14(10), 988-993.

<u>Wayment-Steele, H. K.,</u> Pande, V. S. (2018). Variational encoding of protein dynamics benefits from maximizing latent autocorrelation. *The Journal of Chemical Physics*, 149(21), 216101.

Hernandez, C. X.*, <u>Wayment-Steele, H. K.*,</u> Sultan, M. M.*, Husic, B. E., Pande, V. S. (2018). Variational Encoding of Complex Dynamics. *Physical Review E*, 97(6), 062412.

Sultan, M. M., <u>Wayment-Steele, H. K.,</u> Pande, V. S. (2018). Transferable neural networks for enhanced sampling of protein dynamics. *Journal of Chemical Theory and Computation*, 14(4), 1887-1894.

Husic, B. E., McKiernan, K. A., <u>Wayment-Steele, H. K.,</u> Sultan, M. M., Pande, V.S. (2018) A minimum variance clustering approach produces robust and interpretable coarse-grained models. *Journal of Chemical Theory and Computation*, 14(2), 1071-1082.

<u>Wayment-Steele, H. K.,</u> Frenkel, D., Reinhardt, A. (2017) Investigating the role of boundary bricks in DNA brick self-assembly. *Soft Matter* (2017) 13, 1670-1680.

Agnarsson, B., <u>Wayment-Steele, H. K.,</u> Höök, F., Kunze, A. Monitoring of single and double lipid membrane formation with high spatiotemporal resolution using evanescent light scattering microscopy. (2016) *Nanoscale* (8), 19219-19223.

Wayment-Steele, H. K., Jing, Y., Swann, M. J., Johnson L. E., Agnarsson, B., Johal, M. S., Kunze, A. (2016) Effects of Al^{3+} on phosphocholine and phosphoglycerol containing solid supported lipid bilayers. *Langmuir* 32:7, 1771–1781.

Wayment-Steele, H.K., Johnson L. E., Tian, F., Dixon, M. C., Benz, L., Johal, M. S. "Monitoring N3 Dye Adsorption and Desorption on TiO2 surfaces: A combined QCM-D and XPS study." *ACS Applied Materials & Interfaces* (2014) 6, 9093-9099.

Tian, F., Cerro, A.M., Mosier, A. M., Wayment-Steele, H. K., Shine, R. S., Park, A., Webster, E. R., Johnson, L. E., Johal, M. S., Benz, L. (2014) "Surface and Stability characterization of a nanoporous ZIF-8 thin film". *Journal of Physical Chemistry C* 118, 14449-14456.

Invited reviews & book chapters

Wayment-Steele, H.K., Das, R. Learning RNA structure prediction from crowd-designed RNAs. *Nature Methods* 19, 1181–1182 (2022).

Wayment-Steele, H. K., Wu, M., Gotrik, M., Das, R. (2019). Evaluating riboswitch optimality. *Methods in Enzymology*, 623, 417-450.

Teaching

Instructor, Biomolecular NMR course, Swedish NMR Centre, Univ. Gothenburg   Sep. 2023

Co-instructor, Topics in Genomics (BIOL 4013)   Fall 2020
       Co-instructor: Gloria Regisford, Biology Department, Prairie View A & M Univ.
       45 students
- Invited and hosted 7 visiting speakers from historically underrepresented backgrounds
- Developed a novel final project using Eterna as a platform for students to create puzzles based on RNA molecules relevant to health and disease
- Developed interactive class activities on reading scientific literature and introduction to principles in RNA biophysics
- Coordinated interactive career information sessions with volunteer graduate students

Teaching assistant, Macromolecules (BIOC 241)   Fall 2020
       Instructors: Rhiju Das, Pehr Harbury, Biochemistry Dept., Stanford Univ.
       40 students
- Developed and led interactive virtual course sessions once a week
- Held office hours, assisted in grading

Teaching assistant, Thermodynamics (CHEM 175)   Spring 2017
       Instructors: Bianxiao Cui, Will Pfalzgraff, Dept. of Chemistry, Stanford Univ.
       60 students
- Assisted instructors in developing a new computational lab section for the class
- Helped develop lab handouts, code bases and exercises
- Assisted in running and delivering lectures for three weekly lab sections
- Developed homework and exam material, held office hours, assisted in grading

Teaching assistant, Statistical Mechanics (CHEM 171)   Winter 2017
       Instructor: Tom Markland, Dept. of Chemistry, Stanford Univ.
       60 students
- Prepared and delivered weekly hour-long discussion sections to clarify concepts in statistical mechanics
- Developed corresponding activities for discussion sections
- Developed homework and exam material, held office hours, assisted in grading

Teaching assistant, Accelerated Chemical Principles (CHEM 31X)   Fall 2016
       Instructors: W. E. Moerner, Charlie Cox, Dept. of Chemistry, Stanford Univ.

150 students
- Directed two weekly experimental lab sections of 15 students each
- Assisted in writing and developing homework, quizzes, exam materials, held office hours, assisted in grading

Supervisor, Nanotechnology Doctoral Training Centre   Michaelmas 2015
    Cavendish Labs, Cambridge University
    20 students
- Met weekly with groups of first-year PhD students to supervise a theoretical chemistry lab exercise
- Developed course handouts and code for data analysis

Mentorship, Outreach

Program advisor, Undergraduate and DEI education, Nucleate accelerator   2021-2022
- Advised undergraduate and PhD students on initiatives and grants to engage students in biotech-related research.

Program mentor, Center for Genetically Encoded Materials REU, UC Berkeley   Summer 2021
- Mentored 2 undergraduates in projects creating an online database of ribosome studies.

Outreach, Eterna Project, Stanford University   2019-2021
- Mentored PVAMU undergraduates in directed reading projects related to RNA vaccines, graduate school application preparation
- Assisted in writing grants for outreach initiatives
- Assisted in science communication, social media presence, hiring

Program mentor, Stanford Summer Research Program   Summer 2020
- Mentored 1 undergraduate in a data science project interpreting machine learning models for RNA structure prediction

Mentor for Teaching assistants, Department of Chemistry, Stanford University   2017-2018
- Met monthly with 4 graduate teaching assistants per quarter (12 in total) to discuss teaching strategies and help guide goal-setting for teaching
- Each quarter, ran classroom observation sessions, coordinated teaching evaluations, and summarized and discussed feedback with each mentee
- Helped plan, coordinate and run weeklong Chemistry department TA training orientation at start of fall quarter
- Developed and ran training sessions on effective teaching strategies and grading

Professional Service

General Chair, "Machine Learning for Structural Biology" workshop at NeurIPS   2023
- Led writing and submission of workshop proposal to NeurIPS (35% acceptance rate)
- Established a novel program working with the journal *PRX Life* to create an option for authors to publish their contributions, with publication fees waived
- Managed selection of invited speakers and fundraising to support travel grants for students

Reviewer   2019-present
- Nature Methods, Nature Communications, PLOS Comp. Bio., Nucleic Acids Research, Vaccines, and more

Organizer, NSF Protein Folding Consortium Conference, Berkeley, CA   Spring 2017

Senator, Stanford Chemistry Student-Hosted Colloquium Committee   2016 – 2018

Invited talks

HHMI award lecture, Quantitative Biology program, Brandeis University. *"Learning the languages of life (Or, why is AlphaFold like ChatGPT?)"*   October 2023

Prairie View A & M University, remote. *"Intro to RNA structure."*   every Fall, 2021-2023

CASP special interest group for ensembles, remote. *"Predicting multiple conformational states using AlphaFold2 and clustering."*   June 7, 2023

Boston Protein Modeling and Design Club, Cambridge, MA. *"Understanding (and discovering?) fold-switching proteins."*   April 12, 2023

Machine Learning for Proteins, remote. *"Understanding fold-switching proteins using AlphaFold2 and sequence clustering."*   April 28, 2023

Relay therapeutics, Cambridge, MA. *"Predicting multiple conformational states by combining AlphaFold2 and sequence clustering."*   Jan. 17, 2023

Pomona College Chemistry Dept, Claremont, CA. *"Inferring RNA structure and stability via high-throughput experiment."*   July 22, 2022

Inceptive Nucleics, remote. *"Inferring RNA structure and stability via high-throughput experiment."*
                    April 13, 2022

Schrödinger Multiscale modelling for biotherapeutics symposium, remote. *"Improving the Stability of mRNA therapeutics through biophysics, machine learning, and crowdsourcing."*   May 13, 2021

TEDx Washington High, Fremont, CA. *"Designing stabilized vaccines with community science."*
                    May 1, 2021

Center for HIV-1 Studies Annual Workshop, remote. *"Inferring RNA ensembles via high-throughput data."*
                    April 5, 2021

IEEE Silicon Valley Chapter, Information Theory Society. *"Improving the stability of mRNA therapeutics."*
                    March 24, 2021

Conference Presentations (Contributed)

"Computational Aspects of Biomolecular NMR" Gordon Research Conference, Mt. Snow, VT. *"Have protein language models learned dynamics? Evaluating with a large-scale benchmark of NMR relaxation data."*
                    June 20, 2023

Machine Learning in Structural Biology workshop, Neural Information Processing Systems conference, New Orleans, LA. *"Predicting conformational landscapes of known and putative fold-switching proteins using AlphaFold2"*   Dec 3, 2022

International Conference on Intelligent Systems for Molecular Biology (ISMB). *"Improving RNA structure prediction with high-throughput crowdsourced data."*   July 13, 2020

Media engagement

Nature. *"Remarkable AI tool designs mRNA vaccines that are more potent and stable."*   May 2, 2023

Fifty Years Podcast. *"Screening for Enhanced RNA Vaccines with Kathrin Leppek, Gun Woo Byeon, and Hannah Wayment-Steele."*   October 14, 2021

National Geographic. *"Future COVID-19 vaccines might not have to be kept so cold."*   April 13, 2021

Patent Applications

H. K. Wayment-Steele, E. Sharma, R. Das, W. Greenleaf. 63/245,744, "Systems and Methods to Determine Nucleic Acid Thermodynamics and Uses thereof", Sep. 17, 2021.

R. Das, H. K. Wayment-Steele. PCT/US2021/040026, "Systems and Methods to Enhance RNA Stability and Translation and Uses Thereof", July 1, 2021.

R. Das, C. A. Choe, H. K. Wayment-Steele, W. Kladwang, 17/364,890, "Systems and Methods to Enhance RNA Stability and Translation and Uses Thereof", June 30, 2021.