Hannah K. Wayment-Steele
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I integrate deep learning, bioinformatics, and nuclear magnetic resonance spectroscopy to advance methods to predict protein dynamics. I am interested in ultimately gaining a complete understanding of protein evolution, starting from the DNA level.

Education

Postdoc, Biochemistry, Brandeis University 2022 – present
Advisor: Dorothee Kern
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

Research

Jane Coffin Childs Postdoctoral Fellow, Brandeis University 2022 – present
- Developed deep-learning-based approaches to predict multiple conformational states in proteins.
- Developed 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
- Consulted on projects using deep learning in structural biology and biotechnology.

Postdoctoral Fellow, Wyss Institute, Harvard Medical School 2021 – 2022
- 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.

Manuscripts Under Review (*Equal contributions)

Wayment-Steele, H.K.*, Ojoawo, A.*, Otten, R., Apitz, J.M., Pitsawong, W., Ovchinnikov, S., Colwell, L.J., Kern, D. "Prediction of multiple conformational states via sequence clustering and AlphaFold2". Preprint: *bioRxiv* 2022.10.17.512570.

Peer-Reviewed Publications

Wayment-Steele, H. K.*, 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.

Wayment-Steele, H.K., 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.*, Wayment-Steele, H. K.*, 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., Wayment-Steele, H. K., 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.

Wayment-Steele, H.K., 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., Wayment-Steele, H. K., 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.

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

Sultan, M. M., Wayment-Steele, H. K., 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., Wayment-Steele, H. K., 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.

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

Agnarsson, B., Wayment-Steele, H. K., 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.

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 2015
Awarded to one Pomona College graduate annually in the natural sciences who exhibits the highest academic promise.
Beckman Scholar 2014
Goldwater Scholar 2014

Professional Service

General Chair, "Machine Learning for Structural Biology" workshop at NeurIPS 2023
Reviewer 2019-present
- Nature Methods, Nature Communications, 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

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 lead, Eterna Project, Stanford University 2019-2021
- Mentored PVAMU undergraduates in directed reading projects related to RNA vaccines, graduate school application preparation.
- Invited and coordinated 8 guest lecturers for partnership with Prairie View A&M University BIOL 4013.
- 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. Specifically, developed and ran training sessions on effective teaching strategies and grading.

Teaching

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

Volunteer co-instructor, Topics in Genomics (BIOL 4013) Fall 2020
Co-instructor: Gloria Regisford, Biology Department, Prairie View A & M Univ.
45 students, two TAs.
Invited and hosted 7 visiting speakers from historically underrepresented backgrounds. Developed 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. Graded assignments.

Teaching assistant, Macromolecules (BIOC 241) Fall 2020
Instructors: Rhiju Das, Pehr Harbury, Biochemistry Dept., Stanford Univ.
40 students, one of 3 TAs
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, single TA
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.
In a non-mandatory course review (13 respondents), 54% said my instruction was "extremely effective", 31% said "very effective". 46% said they learned "a great deal" from my teaching, 31% said they learned "a lot".

Teaching assistant, Statistical Mechanics (CHEM 171) Winter 2017
Instructor: Tom Markland, Dept. of Chemistry, Stanford Univ.
60 students, one of two TAs
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, one of 6 TAs
Directed two weekly experimental lab sections of 15 students each. Assisted in writing and developing homework, quizzes, exam materials, held regular office hours, graded all materials for sections.

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

Invited talks

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

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.