Hannah K. Wayment-Steele

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Education

Ph.D. Student in Chemistry, Stanford University — Anticipated 2021
Concentration in Chemical Physics
Supervisor: Rhiju Das

M.Phil. in Chemistry, University of Cambridge — September 2016
Supervisor: Daan Frenkel
Funded by the Churchill Scholarship
Thesis: Investigating the Role of Boundary Bricks in DNA Brick Assembly via Monte Carlo Simulation

B.A., Pomona College — May 2015
Chemistry and Applied Mathematics (Double Major), Minor in Music
GPA: 3.93, Magna cum Laude
Chemistry Thesis: Investigating the Effect of Al^{3+} on Lipid Bilayers: Experimental and Simulation Studies
Mathematics Thesis: A Stochastic Differential Equations Model for Microtubule Dynamics in Early *C. Elegans* Development

Scholarships & Awards

NSF Graduate Research Fellowship — April 2016
Churchill Scholarship, Sir Winston Churchill Foundation of the USA — January 2015
John Stauffer Prize for Academic Merit in the Sciences, Pomona College — May 2015
– *Awarded to one senior annually in the natural sciences who exhibits the highest academic promise.*
Philip Goldberg Memorial Prize — May 2015
– *Awarded to one student annually for outstanding musical performance.*
Beckman Scholar — April 2014
Goldwater Scholar — March 2014
ACS Colloid & Surface Chemistry Division Poster Award — March 2014
Tileston Physics Prize — August 2014
National Merit Scholar — March 2011
Siemens Award for Advanced Placement — February 2011

Peer Reviewed Publications

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

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*, 1-6.

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

C. X. Hernàndez*, H. K. Wayment-Steele*, M. M. Sultan*, B. E. Husic, V. S. Pande (2018). Varia-

tional Encoding of Complex Dynamics. *Physical Review E* *Equal contributions.

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

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

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

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

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

H. K. Wayment-Steele, L. E. Johnson, F. Tian, M. C. Dixon, L. Benz and M. S. Johal. "Monitoring N3 Dye Adsorption and Desorption on TiO_2 Surfaces: A Combined QCM-D and XPS Study." *ACS Applied Materials & Interfaces* (2014) 6, 9093-9099.

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

Research Experience

Das Group August 2018 to present

Department of Biochemistry, Stanford University

- Developed metrics, criteria and benchmark datasets to evaluate all commonly-used physics-based RNA secondary structure prediction algorithms on likelihood prediction of chemical mapping data, accuracy of predicting riboswitch fold changes. Also developed updated benchmark datasets for single-structure accuracy prediction.
- Developed a statistical inference model to train on novel forms of structural data and demonstrated that accuracy on these novel measures was improved.
- Reviewed all synthetic riboswitches and evaluated their performance based on a measure for optimality developed by colleagues.
- Analyzed high-throughput riboswitch experiments using unsupervised learning methods, visualized results from large datasets, and communicated results for publications and to citizen scientist collaborators.

Pande Group September 2016 to August 2018

Department of Chemistry, Stanford University

- Developed an unsupervised learning framework (the Variational Dynamics Encoder, VDE) to encode time-series data with the purpose of extracting protein dynamic motions from all-atom molecular dynamics simulation data and applying via transfer learning to related systems.
- Performed structural modeling and enhanced sampling simulations of protein-protein and ligand-protein interactions in collaboration with Terence Strick and Charlie Gosse (INSERM, PSL University) to develop a novel single-molecule scaffold for measuring affinity.
- Developed a featurization method to more interpretably represent intrinsically disordered proteins (IDPs) in terms of their transient secondary structure to build Markov State Models (MSMs) of IDPs.

- Helped develop a more robust microstate clustering technique to create more interpretable MSMs.

Frenkel Group September 2015 to September 2016
Department of Chemistry, University of Cambridge

- Performed Monte Carlo simulations of self-assembling DNA strands with the intent of understanding kinetic traps and nucleation pathways in addressable self-assembly.
- Implemented simulations in other thermodynamic ensembles for the above system.

Johal Group January 2012 to present
Pomona College Chemistry Department

- Designed and performed experiments to characterize dye adsorption to semiconductors for applications in Dye-Sensitized Solar Cells.
- Conducted Molecular Dynamics simulations of metal ions and lipid membranes.
- Collaborated in experiments to characterize the physical properties of immobilized ZIF-8 nanoparticles.
- Mentored undergraduate researchers on surface chemistry projects including studying the effects of metal ions on lipid membranes, adsorption of organic dyes for photovoltaics, and effects of anti-microbial peptides on lipid membranes.

Biological Physics Department May-July 2013 and 2014
Chalmers Institute of Technology, Gothenburg, Sweden

- Designed and performed experiments to investigate the effects of both biologically-relevant and neurotoxic metal ions on physical properties of model lipid membranes using surface techniques including Quartz Crystal Microbalance with Dissipation Monitoring (QCM-D), Dual Polarization Interferometry (DPI), and Fluorescence Recovery after Photobleaching (FRAP).

Selected Oral Presentations

H. K. Wayment-Steele. "An Interpretable Model for the p53-CTD Disordered Landscape." Biophysical Society Annual Meeting, San Francisco, CA, 21 Feb. 2018.

H. K. Wayment-Steele. "Investigating Effects of Al^{3+} on Structure and Fluidity of Lipid Membranes: FRAP and Molecular Dynamics." American Chemical Society National Conference, Denver, CO, 3/22/2015.

H. K. Wayment-Steele, L. E. Johnson, M. C. Dixon, M. S. Johal. "Characterization of N3 Dye Adsorption on TiO_2 using QCM-D," SPIE Solar Energy & Technology conference, San Diego, CA, 8/25/2013.

Selected Poster Presentations

H. K. Wayment-Steele, C. X. Hernandez, B. E. Husic, V. S. Pande. "Hierarchical Clustering of Markov State Models Reveals Sequence Effects in p53-CTD Dynamic Behavior". GRC "Proteins" 2017, Holderness, NH.

H. K. Wayment-Steele, L. E. Johnson, S. Svedhem, M. S. Johal, B. Kasemo, A. Kunze. "Investigating Effects of Al^{3+} on Lipid Membranes: FRAP and Molecular Dynamics," International Conference on Nanoscience and Technology, American Vacuum Society, 7/20/2014.

H. K. Wayment-Steele A. Kunze, L. E. Johnson, M. S. Johal, S. Svedhem. "QCM-D and MD Study of Al^{3+} Effects on Membrane Structure," American Chemical Society National Meeting, Dallas, TX, 4/16/2014.
Poster Award, ACS Colloids and Surface Chemistry Division

Invited Workshops

D. E. Shaw Research Graduate and Postdoc Women's Forum — June 2017
New York City, NY

MolSim: Advanced Molecular Simulation — January 2016
Amsterdam, Netherlands

Telluride School of Theoretical Chemistry — July 2015
Telluride, CO

Conference Proceedings

H. K. Wayment-Steele, S. Svedhem, L. E. Johnson, M. S. Johal, B. Agnarsson, and A. Kunze (presenting). "Al^{3+} binding effects on lipid membrane structure" German Physical Society Annual Meeting, Berlin, Germany, 3/18/2015.

M. C. Dixon (presenting), H. K. Wayment-Steele, L. E. Johnson, F. Tian, L. Benz, and M. S. Johal. "Fundamental Dye Self-assembly and Removal Studies". Smart Coatings Conference, Orlando, FL, 2/25/2015.

B. Agnarsson, H. K. Wayment-Steele, S. Svedhem, F. Höök, B. Kasemo, and A. Kunze (presenting). "Ion-mediated formation of a double lipid membrane." German Biophysical Society Annual Meeting, Lübeck, Germany, 9/14/2014.

H. K. Wayment-Steele, L. E. Johnson, M. C. Dixon, M. S. Johal. (2013, September 13). "Characterization of N3 Dye Adsorption on TiO_2 using Quartz-Crystal Microbalance with Dissipation Monitoring." In L. Eldada, M. Heben (Eds.) *SPIE Proceedings Vol. 8823.* Paper Presented at SPIE Optics & Photonics: Thin Film Solar Technology V, San Diego, 25-29 August.

Science Writing and Outreach experience

Member of organization commitee — June 2017
Protein Folding Consortium Workshop, Berkeley, CA

Contributing writer — October 2015-August 2016
Cambridge University BlueSci Magazine
- Contributed regular science news briefs.
- Featured longform piece: H. K. Wayment-Steele, "The *Wunderkammer*: The Dawn of Curiosity in Europe", Cambridge University BlueSci Magazine (2016) 35, 30-31.

Head Student Liaison — August 2013 to June 2015
Pomona College Chemistry Department

Co-President, Food Science Club — May 2014 to June 2015
Pomona College

Teaching Experience

Teaching Assistant: Physical Chemistry I — Spring 2017
Bianxiao Cui, Department of Chemistry, Stanford University
- Assisted in developing and running weekly discussion sections and office hours.
- Helped write and grade homeworks, midterms, exams.

Teaching Assistant: Physical Chemistry III — Winter 2017
Tom Markland, Department of Chemistry, Stanford University
- Developed material to aid understanding in weekly discussion sections and gave lectures.

- Helped develop and grade homeworks, midterms, exams.

Teaching Assistant: Accelerated Chemical Principles Fall 2016
W.E. Moerner, Charles Cox, Department of Chemistry, Stanford University
- Supervised weekly laboratory sections and office hours.
- Helped develop laboratory section materials and exam questions.

Practical Supervisor Fall 2015
NanoDTC, Cavendish Laboratory, Cambridge
- Met weekly with first-year PhD students to supervise a practical in Monte Carlo simulation of DNA brick self-assembly.
- Developed course handouts and code for data analysis.

Instructor: Directed Study in Computational Chemistry Spring/Summer 2015
Malkiat Johal, Pomona College Chemistry Department

Laboratory Assistant: Physical Chemistry –Thermodynamics Spring 2015
Mukesh Arora, Pomona College Chemistry Department

Teaching Assistant: Physical Chemistry for Molecular Biology Spring 2015
Malkiat Johal, Pomona College Chemistry Department

Teaching Assistant: Differential Equations Spring 2014
Dashiel Fryer, Pomona College Math Department

Teaching Assistant: Physical Chemistry –Quantum Mechanics Fall 2014
Malkiat Johal, Pomona College Chemistry Department

Grader: Linear Algebra Fall 2012
Shahriar Shahriari, Pomona College Math Department

Memberships

Phi Beta Kappa April 2015
Mortar Board April 2014
Sigma Xi Scientific Research Society August 2013