Hannah K. Wayment-Steele

333 Campus Drive, Stanford, CA 93405
hannahw1@stanford.edu
hwaymentsteele.github.io

Education

Ph.D. Student in Chemistry, Stanford University — Anticipated 2021
Concentration in Chemical Physics
Supervisor: Vijay S. Pande

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

Manuscripts under Review

H. K. Wayment-Steele V. S. Pande (2018). Note: Variational Encoding of Protein Dynamics Benefits from Maximizing Latent Autocorrelation. arXiv preprint arXiv:1803.06449.

C. X. Hernàndez*, H. K. Wayment-Steele*, M. M. Sultan*, B. E. Husic, V. S. Pande (2017). Variational Encoding of Complex Dynamics. arXiv preprint arXiv:1711.08576. *Equal contributions.

Peer Reviewed Publications

M. M. Sultan, H. K. Wayment-Steele, V. S. Pande (2018). Transferable neural networks for enhanced sampling of protein dynamics. arXiv preprint arXiv:1801.00636.

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, 17711781.

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

Pande Group September 2016 to present
Department of Chemistry, Stanford University

- Helped develop 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.
- Developed methods to apply the VDE to perform enhanced sampling on proteins for the purpose of more rapidly simulating perturbations to a system.
- 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.
- Collaborated with experimentalists and ran enhanced sampling simulations of their proprietary system.

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.
- Developed code implementing the Grand Canonical ensemble for the above system.

Johal Group January 2012 to present
Pomona College Chemistry Department

- Developed 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 in GROMACS.
- Collaborated on a series of experiments to characterize the physical properties of ZIF-8 nanoparticles immobilized on silicon and gold surfaces.
- Mentored other undergraduate researchers on projects related to 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

- Developed and performed experiments to investigate the effects of Ca^{2+}, Mg^{2+}, and Al^{3+} on physical properties of model lipid membranes using techniques including Quartz Crystal Microbalance with Dissipation Monitoring (QCM-D), Dual Polarization Interferometry (DPI), and Fluorescence Recovery after Photobleaching (FRAP).
- Advised other researchers on QCM-D experiments investigating ion-membrane interactions.

Workshops

D. E. Shaw Research Graduate and Postdoc Womens Forum June 2017
New York City, NY

MolSim: Advanced Molecular Simulation January 2016
Amsterdam, Netherlands

Telluride School of Theoretical Chemistry July 2015
Telluride, CO

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. "Effects of Al^{3+} on Supported Lipid Membranes." DPI/QCM-D User Meeting, Manchester, UK, 10/26/2015.

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

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 Publications

H. K. Wayment-Steele, "The *Wunderkammer*: The Dawn of Curiosity in Europe", Cambridge University BlueSci Magazine (2016) 35, 30-31.

Contributed regular science news briefs for Cambridge University BlueSci Magazine, October 2015 to August 2016, www.bluesci.co.uk.

H. K. Wayment-Steele, L.E. Johnson, M.S. Johal, Solutions manual for *Understanding Nanomaterials*, in preparation.

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.

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

Science Outreach Experience

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

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

- Invited and hosted my international research collaborators as visiting speakers to share research with the Pomona community, meet students, and build relationships with faculty.
- Assisted in hosting candidates during faculty searches.
- Helped plan and organize events for chemistry students at Pomona, contacted outside offices and distributed information to chemistry majors regarding mentoring, course selection, etc.

Tutor in Computational Chemistry Spring 2015
Met weekly with first-year students to teach them principles of Computational Chemistry and introduce them to Molecular Dynamics Research. Developed lesson plans, homework assignments, and readings.

Co-President, Food Science Club May 2014 to June 2015
Helped plan and organize events to excite and educate the Pomona College community about the science of food, taste, cooking, and wine making, including monthly cooking sessions, discussions, and experiments based on chemical and biochemical principles.

Pomona College represenative February 2014
Selected to present my research to HRH Princess Maha Chakri Sirindhorn of Thailand, one of three students to receive the honor.

Assistant organizer October 2014
International Symposium on Biomathematics and Ecology, Claremont, CA