ANDREW L. FERGUSON

204 MSEB (MC-246), 1304 W. Green St., Urbana, IL 61801
tel: (217) 300-2354 | fax: (217) 333-2736 | email: alf@illinois.edu | www: ferguson.matse.illinois.edu

CURRENT POSITION

Assistant Professor of Materials Science and Engineering April 2012 – present
Affiliated Assistant Professor of Chemical and Biomolecular Engineering
Affiliated Assistant Professor of Physics
Affiliated Assistant Professor of Computational Science and Engineering
Faculty Affiliate of Frederick Seitz Materials Research Laboratory
Faculty Affiliate of Carl R. Woese Institute for Genomic Biology
University of Illinois at Urbana-Champaign

RESEARCH INTERESTS

Molecular Simulation | Machine Learning | Self-Assembly | Viral Dynamics | Protein Folding

- Molecular modeling and simulation of biophysical systems at atomistic and coarse-grained resolution
- Systematic order parameter discovery using linear and nonlinear dimensionality reduction tools
- Many-body nonlinear learning for the design of self-assembling soft materials
- Low-dimensional descriptions of viral fitness landscapes and evolutionary dynamics
- Nonlinear inference of protein folding landscapes from univariate time series data
- Molecular simulation of the self-assembly of bioorganic electronic polymers and asphaltenes

EDUCATION

Ragon Postdoctoral Fellow **MIT** Oct 2010 – April 2012
Department of Chemical Engineering – Laboratory for Computational Immunology
Ragon Institute of MGH, MIT, and Harvard
Advisor: Prof. A.K. Chakraborty

- Developed effective Hamiltonian descriptions of HIV fitness to guide next generation vaccine design
- Computational identification of novel broadly neutralizing HIV antibody epitopes by compressed sensing

Ph.D. **Princeton University** Aug 2005 – Sept 2010
Department of Chemical and Biological Engineering
Advisors: Profs. A.Z. Panagiotopoulos, P.G. Debenedetti, and I.G. Kevrekidis
Dissertation: "A Computational Investigation of Low-Dimensional Parametrizations for n-Alkanes and Peptides in Water"

- Developed molecular dynamics simulations to study the *n*-alkane structure-solubility relationship
- Applied diffusion maps to extract dynamic descriptions of *n*-alkane, peptide and dewetting dynamics
- Simulated maturation mechanism of an antimicrobial "lasso" peptide in an experimental collaboration
- Integrated diffusion maps with umbrella sampling in a new protocol for order parameter discovery

M.Eng., ACGI **Imperial College London** Sept 2001 – June 2005
Department of Chemical Engineering and Chemical Technology

- Graduated with first-class honors as top-ranked student in the program
- Completed a final year industrial collaboration with Rolls-Royce Fuel Cell Systems, Derby, UK

M.Eng. **Carnegie Mellon University** Aug 2003 – June 2004
Department of Chemical Engineering

- Selected to participate in junior year exchange as part of Imperial College M.Eng. degree (4.0/4.0)

CONTRIBUTED PRESENTATIONS

21. "Explicit nonlinear collective variables and biased molecular dynamics using autoencoders" AIChE Annual Meeting, San Francisco, CA, November 13-18 2016
20. "Nonlinear learning of colloidal assembly mechanisms from simulation and experiment" AIChE Annual Meeting, San Francisco, CA, November 13-18 2016

19. "Mixing machine learning with experiment: Nonlinear learning of assembly landscapes and mechanisms from particle tracking data" ACS National Meeting – ACS Computers in Chemistry (COMP) symposium: "Designing functional biomaterials: Connecting experiment with theory & simulation", Philadelphia, PA, August 21-25 2016
18. "Machine learning of macromolecular folding funnels from univariate measurements" AIChE Annual Meeting, Salt Lake City, UT, November 8-13 2015
17. "Teaching machines to design self-assembling materials" AIChE Annual Meeting, Salt Lake City, UT, November 8-13 2015
16. "Computational design of hepatitis C virus vaccine immunogens" ACS National Meeting, Boston, MA, August 16-20 2015 [Poster]
15. "Teaching machines to design self assembling materials" Foundations of Molecular Modeling and the Materials Genome (FOMMS), The Resort at the Mountain, Welches, OR, July 12-16 2015 [Poster]
14. "Machine learning in molecular self-assembly, folding, and virology" Machine Learning for Many-Particle Systems, Institute for Pure and Applied Mathematics (IPAM), UCLA, Los Angeles, CA, February 23-27 2015 [Poster]
13. "Computational design of hepatitis C vaccines" AIChE Annual Meeting, Atlanta, GA, November 16-21 2014
12. "Systematic inference of self-assembly pathways by nonlinear machine learning" AIChE Annual Meeting, San Francisco, CA, November 3-8 2013
11. "From viral sequences to fitness landscapes: A new paradigm for *in silico* vaccine design" AIChE Annual Meeting, San Francisco, CA, November 3-8 2013
10. "Water under nanoscopic hydrophobic confinement: Phase behavior, sublimation mechanism, and a novel monolayer ice" Gordon Research Conference – Physics and Chemistry of Liquids, Holderness, NH, August 4-9 2013 [Poster]
9. "Water under nanoscopic hydrophobic confinement: Phase behavior, sublimation mechanism, and a novel monolayer ice" ACS National Meeting, New Orelans, LA, April 7-11 2013
8. "From HIV protein sequences to viral fitness landscapes: A new paradigm for *in silico* vaccine design" AIDS Vaccine 2012, Boston, MA, September 9-12 2012 [Poster]
7. "*In silico* reconstruction of HIV viral fitness landscapes" Biophysical Society Annual Meeting, San Diego, CA, February 25-29 2012 [Poster]
6. "Spin glass models of HIV fitness landscapes" 106th Rutgers Statistical Mechanics Conference, Rutgers, NJ, December 18-20 2011
5. "Integration of umbrella sampling and nonlinear dimensionality reduction using diffusion maps: Iterative determination of the 'right' order parameters" AIChE Annual Meeting, Salt Lake City, UT, November 7-12 2010
4. "Spontaneous lasso formation in pro-microcin J25: Replica exchange molecular dynamics and nonlinear dimensionality reduction" AIChE Annual Meeting, Salt Lake City, UT, November 7-12 2010
3. "Systematic identification of relevant order parameters in biophysical systems" AIChE Annual Meeting, Nashville, TN, November 8–13 2009
2. "Maturation mechanism of microcin J25: Free energy analysis and low-dimensional kinetics from replica exchange molecular dynamics" AIChE Annual Meeting, Nashville, TN, November 8-13 2009
1. "Solubility and molecular conformations of *n*-alkane chains in water" AIChE Annual Meeting, Philadelphia, PA, November 16-21 2008

INVITED TALKS

42. "TBA" Recent Advances in Modeling Rare Events (RARE): Methods and Applications, Jaypee Palace Hotel, Agra, India, December 7-10 2017
41. "TBA" Physical Concepts and Computational Models in Immunology, MIT, Cambridge, MA, October 11-12 2017
40. "Nonlinear reconstruction of viral fitness landscapes and macromolecular folding funnels from experimental data" Center for Biological Physics, Arizona State University, Tempe, AZ, September 27 2017
39. "TBA" Department of Chemistry, Johns Hopkins University, Baltimore, MD, September 12 2017
38. "Machine learning in soft and biological materials: Engineering self-assembling colloids and viral phase behavior" Bioengineering Seminar, UCLA, Los Angeles, CA, June 8 2017
37. "Statistical learning of viral fitness landscapes" Midwest Thermodynamics and Statistical Mechanics Conference, University of Notre Dame, Notre Dame, IN, June 4-6 2017
36. "Machine learning in soft and biological materials: Engineering self-assembling colloids and viral phase behavior" Institute for Molecular Engineering Seminar, University of Chicago, Chicago, IL, May 26 2017

35. "Nonlinear machine learning in soft materials engineering and design" Machine Learning and Data Science in Materials Modeling, Imaging and Applications, APS/CNM Users Meeting, Argonne National Lab, Argonne, IL, May 9 2017
34. "Machine learning in soft and biological materials: Engineering self-assembling colloids and viral phase behavior" Materials Science and Engineering, Georgia Tech, Atlanta, GA, April 10 2017
33. "Nonlinear machine learning in soft materials engineering and design" APS March Meeting symposium: Frontiers of Computational Materials Science, New Orleans, LA, March 13-17 2017
32. "Machine learning in soft and biological materials: Engineering self-assembling colloids and viral phase behavior" Department of Chemical and Biological Engineering Seminar, Princeton University, Princeton, NJ, February 27 2017
31. "Finding folding funnels frae following FRET fluorescence" Third Scottish Chemistry Symposium, Northwestern University, Evanston, IL, January 22-23 2017
30. "Statistical learning of viral fitness landscapes and protein folding funnels" Physical Chemistry Seminar, Department of Chemistry, Purdue University, West Lafayette, IN, January 11 2017
29. "Statistical Learning of Viral Fitness Landscapes for *In Silico* Vaccine Design" CoMSEF Young Investigator Award for Modeling and Simulation – Plenary Talk, AIChE Annual Meeting, San Francisco, CA, November 13-18 2016
28. "Nonlinear reconstruction of hydrophobic folding funnels from experimentally measurable time series" Applied Math Colloquium, Department of Engineering Sciences and Applied Mathematics, Northwestern University, Evanston, IL, October 31, 2016
27. "Statistical learning of viral fitness landscapes for *in silico* vaccine design" Institute for Genomic Biology Seminar, UIUC, Urbana, IL, October 25 2016
26. "Molecular simulation, machine learning, and cheminformatics: Computer-aided design of molecules and vaccines" American Chemical Society (ACS) Student Chapter, UIUC, Urbana, IL, October 19 2016
25. "Statistical learning of viral fitness landscapes and protein folding funnels" Molecular Engineering Seminar, University of Washington, Seattle, WA, October 4 2016
24. "Nonlinear reconstruction of macromolecular folding funnels from univariate time series" ACS National Meeting – ACS Physical Chemistry (PHYS) symposium: Accelerating discovery: Citizen science, big data, and machine learning for physical chemistry, Philadelphia, PA, August 21-25 2016
23. "Direct comparison of experimental and theoretical free energy surfaces for macromolecular folding" CECAM Workshop: Controlling food protein folding and aggregation: Challenges and perspectives in industry, experiments and simulation, Dublin, Ireland, August 18-20 2016
22. "Nonlinear reconstruction of hydrophobic folding funnels from experimentally measurable time series" Telluride Workshop on Hydrophobicity, Telluride, CO, July 12-16 2016
21. "Empirical viral fitness landscapes for rational vaccine design" Department of Microbiology Seminar, UIUC, Urbana, IL, April 21 2016
20. "Computational design of hepatitis C virus vaccine immunogens" National Center for Supercomputing Applications (NCSA) Faculty Fellow Seminar, NCSA, Urbana, IL, April 13 2016
19. "Machine learning of viral fitness landscapes and protein folding funnels" Department of Chemical and Biological Engineering Seminar, SUNY Buffalo, Buffalo, NY, March 23 2016
18. "Machine learning of viral fitness landscapes and protein folding funnels" Department of Chemical and Biomolecular Engineering Seminar, Cornell University, Ithaca, NY, February 29 2016
17. "Machine learning of viral fitness landscapes and protein folding funnels" Department of Materials Science and Engineering Seminar, Boise State University, Boise, ID, January 29 2016
16. "Machine learning of viral fitness landscapes and protein folding funnels" Department of Chemical Engineering Seminar, UT Austin, Austin, TX, January 8 2016
15. "Machine learning of viral fitness landscapes and protein folding funnels" Department of Chemical and Biological Engineering Seminar, Princeton University, Princeton, NJ, December 9 2015
    → Invited and hosted by Chemical Engineering graduate students
14. "Machine learning of materials assembly landscapes and protein folding funnels" Kinetic Networks: From topology to design, Santa Fe Institute Workshop, Santa Fe Institute, Santa Fe, NM, September 17-19 2015 [https://www.youtube.com/watch?v=l6H2GwQxxZg&feature=youtu.be]
13. "The role of machine learning in biophysical assembly and folding" Midwest Computational Biomolecular Modeling Symposium, NIH Center for Macromolecular Modeling and Bioinformatics, UIUC, Urbana, IL, September 15 2015

12. "Machine learning of viral fitness landscapes and protein folding funnels" Computations in Science Seminars, James Franck Institute / MRSEC, University of Chicago, Chicago, IL, May 20 2015
11. "Recovery of single molecule folding landscapes from univariate time series" UIUC Initiative for Mathematical Sciences and Engineering (IMES), Urbana, IL, October 8 2014
10. "Hepatitis C viral fitness landscapes: A paradigm for computational vaccine design" UIUC Biophysics Bootcamp, Urbana, IL, August 21 2014
9. "Computational HIV and HCV vaccine design" UIUC Summer Scholars Institute, Urbana, IL, July 29 2014
8. "Molecular dynamics simulations in ICME" Elements of Integrated Computational Materials Engineering Workshop, Urbana, IL, July 23-25 2014
7. "Hepatitis C viral fitness landscapes and computational vaccine design" Midwest Theoretical Chemistry Conference (MWTCC), Northwestern University, Evanston, IL, June 15-17 2014
6. "Machine learning in soft materials: Protein folding pathways and materials self-assembly mechanisms" UIUC Theoretical and Computational Biophysics (TCB) Colloquium, Urbana, IL, December 6 2013
5. "Teaching machines to design materials and vaccines" Department of Chemical and Biomolecular Engineering Seminar, University of Tennessee, Knoxville, TN, November 26 2013
4. "Teaching machines to design materials and vaccines" Department of Chemical and Biological Engineering Seminar, University of Wisconsin, Madison, WI, November 19 2013
3. "Machine learning in soft materials: Protein folding pathways and materials self-assembly mechanisms" UIUC MechSE Materials Interest Group (MIG) Colloquium, Urbana, IL, October 24 2013
2. "Machine learning and biology: Folding paths and fitness landscapes" UIUC CSE Colloquium, Urbana, IL, February 20 2013
1. "Machine learning and biology: Folding paths and fitness landscapes" UIUC Physics Colloquium, Urbana, IL, November 28 2012

CONFERENCE PAPERS

2. A. Kononov, P. Bellon, T. Bretl, **A.L. Ferguson**, G.L. Herman, K.A. Kilian, J.A. Krogstad, C. Leal, C.R. Maass, A. Schleife, J.K. Shang, D.R. Trinkle, and M. West "Computational Curriculum for MatSE Undergraduates" Paper presented at 2017 American Society for Engineering Education (ASEE) 124th Annual Conference & Exposition, Columbus, OH, June 25-28 2017 [https://peer.asee.org/28060]
1. R.A. Mansbach, G.L. Herman, M. West, D.R. Trinkle, **A.L. Ferguson**, and A. Schleife "WORK IN PROGRESS: Computational Modules for the MatSE Undergraduate Curriculum" American Society for Engineering Education (ASEE) 123rd Annual Conference & Exposition, New Orleans, LA, June 26-29 2016 [http://dx.doi.org/10.18260/p.27214]

BOOK CHAPTERS

1. G.R. Hart and **A.L. Ferguson** "Viral fitness landscapes: A physical sciences perspective" *in* "Systems Immunology: An introduction to modeling methods for scientists" J. Das, C. Jayaprakash (eds.) Taylor and Francis (in press, 2017) [ISBN-10: 1498717403]

PUBLICATIONS

* *Designates corresponding author.*

40. J.Wang and **A.L. Ferguson*** "Nonlinear machine learning in simulations of soft and biological materials" *Mol. Sim.* (submitted, 2017)
→ Invited review article for the "Free Energy Simulations" special issue
39. J. Wang and **A.L. Ferguson** "A study of the morphology, dynamics, and folding pathways of ring polymers with supramolecular topological constraints using molecular simulation and nonlinear manifold learning" *Macromolecules* (submitted, 2017)
38. M.W. Lee, E.Y. Lee, G.H. Lai, N.W. Kennedy, A.E. Posey, W. Xian, **A.L. Ferguson**, R.B. Hill, and G.C.L. Wong "Molecular motor Dnm1 synergistically induces membrane curvature to facilitate mitochondrial fission" *ACS Cent. Sci.* (submitted, 2017)
37. A.W. Long and **A.L. Ferguson*** "Landmark diffusion maps (L-dMaps): Accelerated manifold learning out-of-sample extension" *Appl. Comput. Harmon. Anal.* (in press, 2017) [https://arxiv.org/abs/1706.09396]
36. E.Y. Lee, M.W. Lee, B.M. Fulan, **A.L. Ferguson***, and G.C.L. Wong "What can machine learning do for antimicrobial peptides, and what can antimicrobial peptides do for machine learning?" *Interface Focus* (in press, 2017)

→ *RSC Interface Focus* invited mini-review

35. E.Y. Lee, G.C.L. Wong, and **A.L. Ferguson*** "Machine learning-enabled discovery and design of membrane-active peptides" *Bioorg. Med. Chem.* (in press, 2017) [http://dx.doi.org/10.1016/j.bmc.2017.07.012]
→ Invited mini-review for "Peptide Therapeutics" symposium-in-print
34. Z. Song, R.A. Mansbach, R. Baumgartner, K.-C. Shih, H. He, N. Zheng, X. Ba, Y. Huang, D. Mani, Y. Lin, M.-P. Nieh, **A.L. Ferguson***, L. Yin, and J. Cheng "Modulation of polypeptide conformation through donor-acceptor transformation of side-chain hydrogen bonding ligands" *Nat. Commun.* 92 8 1-8 (2017) [http://dx.doi.org/10.1038/s41467-017-00079-5]
33. W.F. Reinhart, A.W. Long, M.P. Howard, **A.L. Ferguson**, and A.Z. Panagiotopoulos "Machine learning for autonomous crystal structure identification" *Soft Matter* 13 4733-4745 (2017) [http://dx.doi.org/10.1039/c7sm00957g]
32. R.A. Mansbach and **A.L. Ferguson*** "Control of the hierarchical assembly of π-conjugated optoelectronic peptides by pH and flow" *Org. Biomol. Chem.* 15 26 5484-5502 (2017) [http://dx.doi.org/10.1039/C7OB00923B]
→ Invited submission for "Peptide Materials" special issue
→ Selected as 2017 HOT Article in *Organic and Biomolecular Chemistry*
→ Featured as the cover article of *Organic and Biomolecular Chemistry* 15 26 (2017)
31. J. Wang, M. Gayatri, and **A.L. Ferguson*** "Mesoscale simulation and machine learning of asphaltene aggregation phase behavior and molecular assembly landscapes" *J. Phys. Chem. B* 121 18 4923-4944 (2017) [http://dx.doi.org/10.1021/acs.jpcb.7b02574]
30. **A.L. Ferguson*** "BayesWHAM: A Bayesian approach for free energy estimation, reweighting, and uncertainty quantification in the weighted histogram analysis method" *J. Comput. Chem.* 38 18 1583-1605 (2017) [http://dx.doi.org/10.1002/jcc.24800]
29. R.A. Mansbach and **A.L. Ferguson*** "Coarse-grained molecular simulation of the hierarchical self-assembly of π-conjugated optoelectronic peptides" *J. Phys. Chem. B* 121 7 1684–1706 (2017) [http://dx.doi.org/10.1021/acs.jpcb.6b10165]
28. E.Y. Lee, B.M. Fulan, G.C.L. Wong, and **A.L. Ferguson*** "Mapping membrane activity in undiscovered peptide sequence space using machine learning" *Proc. Natl. Acad. Sci. USA* 113 48 13588-13593 (2016) [http://dx.doi.org/10.1073/pnas.1609893113]
27. C.D. Allen, M.Y. Chen, A.Y. Trick, D. Thanh Le, **A.L. Ferguson***, and A.J. Link "Thermal unthreading of the lasso peptides astexin-2 and astexin-3" *ACS Chem. Biol.* 11 11 3043-3051 (2016) [http://dx.doi.org/10.1021/acschembio.6b00588]
26. J. Wang and **A.L. Ferguson*** "Mesoscale simulation of asphaltene aggregation" *J. Phys. Chem. B* 120 32 8016-8035 (2016) [http://dx.doi.org/10.1021/acs.jpcb.6b05925]
25. A.W. Long, C.L. Phillips, E. Jankowski, and **A.L. Ferguson*** "Nonlinear machine learning and design of reconfigurable digital colloids" *Soft Matter* 12 7119-7135 (2016) [http://dx.doi.org/10.1039/C6SM01156J]
24. R.A. Mansbach, **A.L. Ferguson**, K.A. Kilian, J.A. Krogstad, C. Leal, A. Schleife, D.R. Trinkle, M. West, and G.L. Herman "Reforming an undergraduate materials science curriculum with computational modules" *J. Mater. Educ.* 38 3-4 161-174 (2016)
23. J. Hu and **A.L. Ferguson*** "Global graph matching using diffusion maps" *Intelligent Data Analysis* 20 3 637-654 (2016) [http://dx.doi.org/10.3233/IDA-160824]
22. J. Wang and **A.L. Ferguson*** "Nonlinear reconstruction of single-molecule free-energy surfaces from univariate time series" *Phys. Rev. E* 93 032412 (2016) [http://link.aps.org/doi/10.1103/PhysRevE.93.032412]
21. B.A. Thurston, J.D. Tovar, and **A.L. Ferguson*** "Thermodynamics, morphology, and kinetics of early-stage self-assembly of π-conjugated oligopeptides" *Mol. Sim.* 42 12 955-975 (2016) [http://dx.doi.org/10.1080/08927022.2015.1125997]
20. G.R. Hart and **A.L. Ferguson*** "Empirical fitness models for hepatitis C virus immunogen design" *Phys. Biol.* 12 066006 (2015) [http://dx.doi.org/10.1088/1478-3975/12/6/066006]
19. M. Xiong, M.W. Lee, R. Mansbach, Z. Song, Y. Bao, R.M. Peek Jr., C. Yao, L.-F. Chen, **A.L. Ferguson***, G.C.L. Wong, and J. Cheng "Helical antimicrobial polypeptides with radial amphiphilicity" *Proc. Natl. Acad. Sci. USA* 112 43 13155-13160 (2015) [http://dx.doi.org/10.1073/pnas.1507893112]
18. A.W. Long, J. Zhang, S. Granick, and **A.L. Ferguson*** "Machine learning assembly landscapes from particle tracking data" *Soft Matter* 11 8141-8153 (2015) [http://dx.doi.org/10.1039/C5SM01981H]
17. R.A. Mansbach and **A.L. Ferguson*** "Machine learning of single molecule free energy surfaces and the impact of chemistry and environment upon structure and dynamics" *J. Chem. Phys.* 142 105101 (2015) [http://dx.doi.org/10.1063/1.4914144]

→ Ranked as one of the most read *Biological Molecules and Networks* articles of the year

16. G.R. Hart and **A.L. Ferguson*** "Error catastrophe and phase transition in the empirical fitness landscape of HIV" *Phys. Rev. E* 91 032705 (2015) [http://dx.doi.org/10.1103/PhysRevE.91.032705]
15. L. Tang, X. Yang, I. Chaudhury, C. Yao, Q. Yin, Q. Zhou, M. Kwon, L.W. Dobrucki, L.B. Borst, S. Lezmi, W.G. Helferich, **A.L. Ferguson***, T.M. Fan and J. Cheng "Investigating the optimal size of anticancer nanomedicine" *Proc. Natl. Acad. Sci. USA* 111 (43) 15344-15349 (2014) [http://www.dx.doi.org/10.1073/pnas.1411499111]
14. B.D. Wall, Y. Zhou, S. Mei, H.A.M. Ardoña, **A.L. Ferguson** and J.D. Tovar "Variation of formal hydrogen bonding networks within electronically delocalized pi-conjugated oligopeptide nanostructures" *Langmuir* 30 (38) 11375–11385 (2014) [http://www.dx.doi.org/10.1021/la501999g]
13. J.K. Mann, J.P. Barton, **A.L. Ferguson**, S. Omarjee, B.D. Walker, A.K. Chakraborty and T. Ndung'u "The fitness landscape of HIV-1 gag: Advanced modeling approaches and validation of model predictions by in vitro testing" *PLOS Comput. Biol.* 10 8 e1003776 (2014) [http://dx.doi.org/10.1371/journal.pcbi.1003776]
12. B.D. Wall, A.E. Zacca, A.M. Sanders, W.L. Wilson, **A.L. Ferguson** and J.D. Tovar "Supramolecular polymorphism: Tunable electronic interactions within pi-conjugated peptide nanostructures dictated by primary amino acid sequence" *Langmuir* 30 20 5946-5956 (2014) [http://dx.doi.org/10.1021/la500222y]
11. A.W. Long and **A.L. Ferguson*** "Nonlinear machine learning of patchy colloid self-assembly mechanisms and pathways" *J. Phys. Chem. B* 118 15 4228-4244 (2014) [http://dx.doi.org/10.1021/jp500350b]
10. K. Shekhar, C.F. Ruberman, **A.L. Ferguson**, J.P. Barton, M. Kardar, A.K. Chakraborty "Spin models inferred from patient-derived viral sequence data faithfully describe HIV fitness landscapes" *Phys. Rev. E* 88 062705 (2013) [http://dx.doi.org/10.1103/PhysRevE.88.062705]
9. **A.L. Ferguson**, E. Falkowska, L.M. Walker, M.S. Seaman, D.R. Burton and A.K. Chakraborty "Computational prediction of broadly neutralizing HIV-1 antibody epitopes from neutralization activity data" *PLOS ONE* 8 12 e80562 (2013) [http://dx.doi.org/10.1371/journal.pone.0080562]
8. **A.L. Ferguson**, J.K. Mann, S. Omarjee, T. Ndung'u, B.D. Walker and A.K. Chakraborty "Translating HIV sequences into quantitative fitness landscapes predicts viral vulnerabilities for rational immunogen design" *Immunity* 38 606-617 (2013) [http://dx.doi.org/10.1016/j.immuni.2012.11.022]
   → Highlighted in an accompanying commentary article: N. Goonetilleke and A.J. McMichael "HIV-1 vaccines: Let's get physical" *Immunity* 38 410-413 (2013)
   → Editorial selection as feature in Cell "Select" series on antiviral strategies in *Cell* 153 4 (2013)
7. **A.L. Ferguson***, N. Giovambattista, P.J. Rossky, A.Z. Panagiotopoulos and P.G. Debenedetti "A computational investigation of the phase behavior and capillary sublimation of water confined between nanoscale hydrophobic plates" *J. Chem. Phys.* 137 144501 (2012) [http://dx.doi.org/10.1063/1.4755750]
   → Featured as the cover article of Journal of Chemical Physics 137 (2012)
   → Most read regular Journal of Chemical Physics article in October 2012
   → Selected as a 2012 Journal of Chemical Physics Editor's Choice article
6. **A.L. Ferguson**, A.Z. Panagiotopoulos, I.G. Kevrekidis and P.G. Debenedetti "Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach" *Chem. Phys. Lett. Frontiers* 509 1 1-11 (2011) [http://dx.doi.org/10.1016/j.cplett.2011.04.066]
   → Featured as the cover article of Chemical Physics Letters 509 1 (2011)
5. **A.L. Ferguson***, A.Z. Panagiotopoulos, P.G. Debenedetti and I.G. Kevrekidis "Integrating diffusion maps with umbrella sampling: Application to alanine dipeptide" *J. Chem. Phys.* 134 135103 (2011) [http://dx.doi.org/10.1063/1.3574394]
4. **A.L. Ferguson**, S. Zhang, I. Dikiy, A.Z. Panagiotopoulos, P.G. Debenedetti and A.J. Link "An experimental and computational investigation of lasso formation in microcin J25" *Biophys. J.* 99 9 3056-3065 (2010) [http://dx.doi.org/10.1016/j.bpj.2010.08.073]
3. **A.L. Ferguson**, A.Z. Panagiotopoulos, P.G. Debenedetti and I.G. Kevrekidis "Systematic determination of order parameters for chain dynamics using diffusion maps" *Proc. Natl. Acad. Sci. USA* 107 31 13597-13602 (2010) [http://dx.doi.org/10.1073/pnas.1003293107]
2. **A.L. Ferguson**, P.G. Debenedetti and A.Z. Panagiotopoulos "Solubility and molecular conformations of *n*-alkane chains in water" *J. Phys. Chem. B* 113 18 6405-6414 (2009) [http://dx.doi.org/10.1021/jp811229q]
1. E. Guibal, T. Vincent, E. Touraud, S. Colombo, and **A.L. Ferguson** "Oxidation of hydroquinone to *p*-benzoquinone catalyzed by Cu(II) supported on chitosan flakes" *J. Appl. Polym. Sci.* 100 3034-3043 (2006) [http://dx.doi.org/10.1002/app.23702]

TEACHING

ENG 198 – Grand Challenges UIUC 2012, 13, 14

Freshman enrichment elective guiding teams in the study of one of the NAE Grand Challenges

MSE 458 – Polymer Physics UIUC 2013, 14, 15, 16, 17
Intermediate-level introduction to the equilibrium physics and physical chemistry of polymer systems

MSE 498 – Computational Materials Science and Engineering UIUC 2013, 14, 15
MSE 404 – Computational Materials Science and Engineering UIUC 2016
A new course providing hands-on experience with software tools for electronic structure calculations, molecular simulations, finite element modeling, and phase equilibria

Princeton University Preparatory Program Instructor Princeton 2008
Co-designed and co-taught an introductory summer physics course to 20 low-income high-ability high school seniors involving lectures, laboratory work, small group precepts and a field trip

PROFESSIONAL SERVICE

Conference Organization (National)

Aspen Center for Physics 2018 Winter Conference: Aspen, CO
"Data-driven Discovery and Design in Soft and Biological Materials" January 7-13 2018
- Co-organizer with Erik Luijten (MSE, Northwestern) and Gerard Wong (BioE, UCLA)
- Conference to bring together researchers interested in data-driven materials discovery in soft and biological materials to define and codify the key directions, objectives, and methodologies for the field

AIChE CoMSEF Liaison Director 2016-2018
- Facilitate CoMSEF programming and sponsorship, and communicating and advocating activities
- Elected by CoMSEF membership for a 2 year term

AIChE Area 1a Programming Committee 2015-2017
- Responsible for sponsoring symposia, programming, and keynotes at AIChE meetings
- Elected by active committee members of Area 1a: Thermodynamics and Transport Properties

AIChE Annual Meeting 2017 Session Organizer Minneapolis, MN
01A11 – Thermodynamics of Biomolecular Folding and Assembly Oct 29 – Nov 3 2017
21010/12 – Data Mining and Machine Learning in Molecular Sciences I & II

AIChE Annual Meeting 2016 Session Organizer San Francisco, CA
01A14 – Thermodynamics of Biomolecular Folding and Assembly November 13-18 2016
21004 – Data Mining and Machine Learning in Molecular Sciences I & II
21000 – Data-Driven Screening of Chemical and Materials Space

AIChE Annual Meeting 2015 Session Organizer Salt Lake City, UT
01A04 – Thermodynamics of Biomolecular Folding and Assembly November 8-13 2015
21000 – Data Mining and Machine Learning in Molecular Sciences I & II (new session devised by ALF)

AIChE Annual Meeting 2014 Session Organizer Atlanta, GA
706 – Thermodynamics of Biomolecular Folding and Assembly November 16-21 2014

Conference Organization (Regional)

3rd Semi-Annual Midwestern Quantitative Biology (MidQBio) Symposium UIUC
Co-organizer w/ Seppe Kuehn April 9 2016
- Bringing together invited speakers from quantitative biology labs throughout the Midwest
- Student and post-doc "lighting talks" to advertise research and present new results

Computational Science & Engineering Program Annual Meeting UIUC
Co-organizer April 10-11 2014
- Celebration of the 30th anniversary of the Computational Science and Engineering program at UIUC
- Invited speakers from across the US, poster session, graduate fellowship awards

Journal Advisory Boards

Molecular Systems Design and Engineering (RSC, IChemE) 2017 – present

Mentorship and Outreach

Worldwide Youth in Science and Engineering Summer Camp UIUC
Instructor Summer 2013, 2014
- Developed and led a hands-on workshop introducing material science to high school sophomore campers

Illinois Promise Mentor UIUC

Mentor Fall 2013 – present

- Faculty mentor to low-income, high-achieving Illinois Promise undergraduates

Grad Mentoring @ Illinois UIUC
Mentor Fall 2012 – Spring 2014

- Selected as a faculty mentor for traditionally underrepresented graduate students

Workshops

NRC Workshop on Graduate Education in Chemistry Nat'l Acad. Keck Center
Workshop Participant January 23-24 2012

- Discussion between academic and industrial stakeholders on the state and challenges of US graduate education in chemistry to drive NSF and NIH reports, recommendations, and directions

College of Engineering Office of Research NSF CAREER Proposal Workshop UIUC
Panelist March 31 2016

- Member of a faculty panel sharing advice and experiences in securing NSF CAREER award

National Academies Board on Chemical Sciences and Technology Meeting NAS Building, D.C.
Panelist and Speaker March 3 2017

- Speaker and participant in session "Data Science in the Chemical Sciences"
- Workshop and discussion to determine policy directions for chemical sciences

NSF Workshop: "*Advancing and Accelerating Materials Innovation through the Synergistic Interaction among Computation, Experiment, and Theory*" NSF Headquarters, D.C.
Invited Participant May 18-19 2017

- Discussant and participant in reviewing accomplishments, challenges, and directions in materials engineering

Reviews

Manuscript Reviews

- J. Phys. Chem. (5), J. Chem. Phys. (7), Information Fusion (1), Chem. Phys. (1), Chem. Phys. Lett. (1), J. Mol. Graph. Model. (3), J. Chem. Eng. Data (1), Soft Matter (3), J. R. Soc. Interface (1), PLOS ONE (1), Physical Biology (1), J. Phys. D (1), PNAS (3), Langmuir (1), Molecular Modeling and Simulation (1), npj Computational Materials (1), J. Polymer Science (1), Chem (1), Macromolecules (2), Protein and Cell (1), J. Process Control (1), J. Comput. Phys. (1), Nanoscale (1), Mol. Sim. (1), Mol. Sys. Des. Eng. (1), J. Supercrit. Fluids. (1), PLOS Comput. Biol. (1), AIMS Materials Science (1), Nat. Commun. (1), Energy & Fuels (1), eLife (1 - guest editor)

Proposal Reviews

Mail-in:

- NSF: DBI (1), DMR (11), CHE (3), ACI (2) *including* Postdoctoral Research Fellowship in Biology (PRFB) (1), RUI (1), CAREER (3), CDS&E (1), DIBB (2)
- Biotechnology and Biological Sciences Research Council (BBSRC) (2)
- ACS PRF (3)
- amfAR, The Foundation for AIDS Research (6)
- Research Foundation – Flanders (Belgium): Odysseus project (1)
- Technical book proposals: CRC Press (Taylor and Francis) (2), Wiley (1)

Panel:

- NSF: CHE/CTMC (1)

Award Reviews

- ACS COMP Chemical Computing Group Excellence Award for Graduate Students (10)
- National Center for Supercomputing Applications (NCSA) Faculty Fellows Program (4)
- AIChE CoMSEF Graduate Student Awards in Computational Molecular Science and Engineering (15)

Online Educational Content

Elements of Integrated Computational Materials Engineering – Molecular Dynamics with LAMMPS

- Lecture: http://youtu.be/TTDXJXJJi18 (15k+ views) Course Materials: http://uiuc-cse.github.io/icme-su14/

MSE 498 – Computational Materials Science and Engineering

- Lectures and Course Materials: https://nanohub.org/resources/22124

ACADEMIC HONORS AND AWARDS

List of Teachers Ranked Outstanding by their Students	UIUC	2017 (Spring)
Dean's Award for Excellence in Research	UIUC	2017
AIChE CoMSEF Young Investigator Award for Modeling & Simulation	UIUC	2016
List of Teachers Ranked Outstanding by their Students (Top 10%)	UIUC	2016 (Fall)
List of Teachers Ranked Outstanding by their Students (Top 10%)	UIUC	2016 (Spring)
List of Teachers Ranked Outstanding by their Students (Top 10%)	UIUC	2015 (Fall)
ACS COMP OpenEye Outstanding Junior Faculty Award	UIUC	2015 (Fall)
List of Teachers Ranked Outstanding by their Students (Top 10%)	UIUC	2015 (Spring)
National Center for Supercomputing Applications Faculty Fellow	UIUC	2015-16
AIChE nominee for DiscoverE New Faces of Engineering	UIUC	2015
IPAM Conference Travel Award	UIUC	2015
List of Teachers Ranked Excellent by their Students	UIUC	2014 (Fall)
List of Teachers Ranked Excellent by their Students	UIUC	2014 (Spring)
ACS PRF Doctoral New Investigator Award	UIUC	2014
NSF CAREER Award	UIUC	2014
IChemE North America Young Chemical Engineer of the Year	UIUC	2013
Academy for Excellence in Engineering Education Collins Fellow	UIUC	2013
List of Teachers Ranked Excellent by their Students	UIUC	2013 (Fall)
List of Teachers Ranked Excellent by their Students	UIUC	2013 (Spring)
AIDS Vaccine 2012 Conference Scholarship	UIUC	2012
Ragon Institute of MGH, MIT and Harvard Fellowship	MIT	2010 – 2012
William R. Schowalter Travel Award	Princeton	2009
Engineering Council Excellence in Teaching Award	Princeton	2007
SEAS Commendation List for Outstanding Teaching	Princeton	2007
School of Engineering Wu Fellow	Princeton	2005 – 2009
Shell Prize	Imperial College	2005
Governor's Prize in Chemical Engineering	Imperial College	2005
Hinchley Medal for Greatest Merit in Final Examinations	Imperial College	2005
City and Guilds Gold Medal for Excellence	Imperial College	2005
BP Chemicals Prize in Chemical Engineering	Imperial College	2004
Proctor & Gamble Prize for Academic Excellence	Imperial College	2003
Institution of Chemical Engineers Book Prize	Imperial College	2002

PROFESSIONAL AFFILIATIONS

Member of the Institution of Chemical Engineers UK (IChemE)	2001 – present
Member of the American Institute of Chemical Engineers (AIChE)	2008 – present
Member of the American Chemical Society (ACS)	2012 – present
Member of the American Physical Society (APS)	2017 – present

DOCTORAL RESEARCH ADVISEES

Current

Bryce A. Thurston III (Physics, UIUC)	2013 – present
Jiang Wang (Physics, UIUC)	2013 – present
Rachael A. Mansbach (Physics, UIUC)	2014 – present
Wei Chen (Physics, UIUC)	2015 – present
Yutao Ma (Physics, UIUC)	2017 – present

Past

Andrew W. Long (MatSE, UIUC) 2012 – 2017
→ Senior Data Scientist, Business and Safety Graphics Lab, 3M
(Commenced 1 September 2017)

Greg A. Hart (Physics, UIUC) 2012 – 2017
→ Postdoctoral Associate w/ Prof. Jun Deng, Therapeutic Radiology, Yale School of Medicine
(Commenced 1 August 2017)

Benjamin M. Fulan (Math, UIUC)	NSF/MPS/DMS/MCTP PhD research internship	Summer 2014, 15
Matthew R. Ellis (Math, UIUC)	NSF/MPS/DMS/MCTP PhD research internship	Summer 2016

UNDERGRADUATE RESEARCH ADVISEES

Jingtian Hu (MatSE, UIUC)	2012 – 2013
Yuecheng "Peter" Zhou (MatSE, UIUC)	2012 – 2014
Shao Mei (MatSE, UIUC)	2013 – 2014
Alexander Trick (MatSE, UIUC)	2013 – 2016
Ali Hajimirza (CS, U. Oklahoma)	Summer 2013
Abhijit Pujare (EE/CS, Yale)	Summer 2013
Samuel Kaufman (MatSE, UIUC)	2014 – 2015
Deepak Mani (MatSE, UIUC)	2015 – 2017
Bridgette Lafaye (MatSE, UIUC)	2015 – 2017
Suraj Dhanak (MatSE, UIUC)	Summer 2016
Mohit Gayatri (CBE, UIUC)	2016 – present
Chin-Yu "Chester" Cheng (ECE, UIUC)	2016 – present
Aik Rui Tan (MatSE, UIUC)	Summer 2017
Aditi Munshi (CS, Grinnell College)	Summer 2017

RESEARCH SUPPORT

Completed Support

1. DOE/BES, "Self-assembly of Pi-Conjugated Peptides in Aqueous Environments Leading to Energy-Transporting Bioelectronic Nanostructures (Grant No. DE-SC0004857)", PI: J.D. Tovar (Johns Hopkins), Co-PIs: H. Katz (Johns Hopkins), A.L. Ferguson (UIUC), Total Award: $810,000 ($165,407 to Ferguson), 09/01/13 – 08/31/16
2. University of Illinois Initiative for Mathematical Sciences and Engineering (IMSE), "Manifold Learning of Biomolecular Free Energy Surfaces from Noisy Takens' Delay Embeddings", PIs: A.L. Ferguson (UIUC), R.E.L. DeVille (UIUC), Total Award: $5,000, 01/01/14 – 05/15/14
3. University of Illinois College of Engineering, "Strategic Instructional Initiatives Program (SIIP): MatSE Curriculum Reform", PIs: A.L. Ferguson (UIUC), D.R. Trinkle (UIUC), A. Schleife (UIUC), C. Leal (UIUC), Total Award: $89,956 ($5,075 to Ferguson), 06/01/14 – 05/31/15
4. National Center for Supercomputing Applications (NCSA), "Computational Design of Hepatitis C Virus Vaccine Immunogens", PIs: A.L. Ferguson (UIUC), Volodymyr Kindratenko (NCSA/UIUC), Total Award: $25,000 ($25,000 to Ferguson), 06/01/15 – 05/31/16
5. University of Illinois College of Engineering, "Strategic Instructional Initiatives Program (SIIP): MatSE Curriculum Reform", PIs: A.L. Ferguson (UIUC), D.R. Trinkle (UIUC), A. Schleife (UIUC), C. Leal (UIUC), K. Kilian (UIUC), C. Robert E. Maass (UIUC), S.J. Dillon (UIUC), J.A. Krogstad (UIUC), Total Award: $67,630 ($5,536 to Ferguson), 06/01/15 – 05/31/16
6. DOE/BES, "Directed Assembly of Bio-Inspired Supramolecular Materials for Energy Transport and Capture: Mesoscale Construction of Functional Materials in Hydrodynamic Flows (Grant No. DE-SC0011847)", PI: W.L. Wilson (Harvard), Other Senior Personnel: A.L. Ferguson (UIUC), C.M. Schroeder (UIUC), J. Cheng (UIUC), J.D. Tovar (Johns Hopkins), F. Spano (Temple), Total Award: $759,000 ($62,859 to Ferguson), 06/01/14 – 05/31/17
7. University of Illinois College of Engineering, "Strategic Instructional Initiatives Program (SIIP): MatSE Curriculum Reform", PIs: A.L. Ferguson (UIUC), D.R. Trinkle (UIUC), A. Schleife (UIUC), C. Leal (UIUC), C. Robert E. Maass (UIUC), J.A. Krogstad (UIUC), J.K. Shang (UIUC), P. Bellon (UIUC), Total Award: $32,381 ($2,768 to Ferguson), 07/01/16 – 06/30/17

Current Support

1. NSF/DMR/CMMT, "CAREER: Teaching Machines to Design Self-Assembling Materials" (Grant No. DMR-1350008), PI: A.L. Ferguson (UIUC), Total Award: $450,000 ($450,000 to Ferguson), 06/01/14 – 05/31/19
2. American Chemical Society Petroleum Research Fund (ACS-PRF), "Mesoscale Simulation and Machine Learning of Asphaltene Aggregation (Grant No. 54240-DNI6)", PI: A.L. Ferguson, Total Award: $110,000 ($110,000 to Ferguson), 07/01/14 – 08/31/17
3. NSF/ACI/REU, "REU Site: INCLUSION - Incubating a New Community of Leaders Using Software, Inclusion, innovation, interdisciplinary and OpeN-science" (Grant No. ACI-1659702), PI: D. Katz (NCSA/UIUC), Co-PI: O. Kindratenko (NCSA/UIUC), Other Senior Personnel: W.D. Gropp (UIUC), B.A. Grosser (NCSA/UIUC), K. Guan (NCSA/UIUC), K.D. Huff (UIUC), V. Kindratenko (NCSA/UIUC), L.S. Mainzer (NCSA/UIUC), L. Paquette (UIUC), L.-M. Rosu (UIUC), A. Schleife (UIUC), V. Stodden (UIUC), M.J. Turk (UIUC), J. Zhang (UIUC), A. Lipka (UIUC), A.L. Ferguson (UIUC), J. Peng (UIUC), J. Byrd (UIUC), M. Snir (UIUC), Total Award: $360,036, 03/01/17 – 02/28/20

4. NSF/CHE/CTMC, "Nonlinear Dimensionality Reduction and Enhanced Sampling in Molecular Simulation Using Auto-Associative Neural Networks" (Grant No. CHE-1664426), PI: A.L. Ferguson (UIUC), Total Award: $380,105 ($380,105 to Ferguson), 06/15/17 – 05/31/20
5. NSF/MPS/DMS/Mathematical Biology, "Nonlinear Manifold Learning of Protein Folding Funnels From Delay-Embedded Experimental Measurements" (Grant No. DMS-1714212), PI: A.L. Ferguson (UIUC), Total Award: $210,000 ($210,000 to Ferguson), 08/01/17 – 07/31/20
6. NSF/DMR/DMREF, "Self-Assembled Peptide-Pi-Electron Supramolecular Polymers for Bioinspired Energy Harvesting, Transport and Management", PI: J.D. Tovar (JHU), Co-PIs: H.E. Katz, (JHU), A.L. Ferguson (UIUC), Total Award: $1,616,101 ($552,884 to Ferguson), 07/01/17 – 06/30/21 *(Recommended for funding)*
7. NSF/DMR/CMMT, NSF/DMS/Statistics, "MATDAT18: Materials and Data Sciences Hackathon", PI: B. Reich (NCSU), Co-PIs: T. Mueller (JHU), S. Rajasekaran (UConn), A.L. Ferguson (UIUC), Total Award: $148,810 ($9,107 to Ferguson), 08/01/17 – 07/31/18 *(Recommended for funding)*

Pending Support

1. NSF/EEC/NCN, "Network for Computational Nanotechnology – Engineered nanoBIO Node" (Renewal), PI: E. Tajkhorshid (UIUC), Co-PIs: A. Aksimentiev (UIUC), C. Murphy (UIUC), R. Bashir (UIUC), P. Jain (UIUC), Other Senior Personnel: I. Ahmad (UIUC), N. Aluru (UIUC), R. Bhargava (UIUC), Q. Chen (UIUC), J. Cheng (UIUC), B. Cunningham (UIUC), A.L. Ferguson (UIUC), X. Li (UIUC), L. Liu (UIUC), D. Pan (UIUC), U. Ravaioli (UIUC), L.-M. Rosu (UIUC), J. Meza (UC Merced), K. McCloskey (UC Merced), S. Ghosh (UC Merced), A. Boyce (UNC Greensboro), Total Award: $4,000,000, 09/01/17 – 08/31/22
2. NASA, "Universal biology: evolution of complex metabolising systems in the planetary environment", PI: N. Goldenfeld (UIUC), Co-PIs: E. Branscomb (UIUC), I. Caan (UIUC), A.L. Ferguson (UIUC), B. Fouke (UIUC), S. Kuehn (UIUC), T. Kuhlman (UIUC), W.-T. Liu (UIUC), Z. Luthey-Schulten (UIUC), R. Mackie (UIUC), S. Maslov (UIUC), G. Olsen (UIUC), M. Russell (JPL), J. Vallino (Marine Biological Laboratory), C. Werth (UT Austin), S. Dawson (UC Davis), J. O'Dwyer (UIUC), R. Whitaker (UIUC), Total Award: $9,893,001 ($123,690 to Ferguson), 01/01/18 – 12/31/22