ANDREW L. FERGUSON

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ACADEMIC APPOINTMENTS

Professor of Molecular Engineering Feb 2024 – present
Vice Dean for Education and Outreach July 2024 – present
Director of Graduate Studies July 2024 – present
Vice Dean for Equity, Diversity, and Inclusion July 2020 – July 2024
Associate Professor of Molecular Engineering July 2018 – Feb 2024
Pritzker School of Molecular Engineering
University of Chicago

Professor of Chemistry July 2024 – present
Department of Chemistry
University of Chicago

Associate Professor of Materials Science and Engineering Jan 2018 – July 2018
Associate Professor of Chemical and Biomolecular Engineering Jan 2018 – July 2018
Affiliate Associate Professor of Physics Jan 2018 – July 2018
Affiliate Associate Professor of Computational Science and Engineering Jan 2018 – July 2018
University of Illinois at Urbana-Champaign

Faculty Affiliate of National Center for Supercomputing Applications June 2015 – July 2018
Faculty Affiliate of Carl R. Woese Institute for Genomic Biology Nov 2016 – July 2018
Faculty Affiliate of Frederick Seitz Materials Research Laboratory July 2017 – July 2018
Faculty Affiliate of Beckman Institute Aug 2017 – July 2018
University of Illinois at Urbana-Champaign

Assistant Professor of Materials Science and Engineering April 2012 – Jan 2018
Affiliate Assistant Professor of Computational Science and Engineering May 2012 – Jan 2018
Affiliate Assistant Professor of Chemical and Biomolecular Engineering Aug 2013 – Jan 2018
Affiliate Assistant Professor of Physics July 2017 – Jan 2018
University of Illinois at Urbana-Champaign

RESEARCH INTERESTS

Molecular Simulation | Machine Learning | Molecular Design | Self-Assembly | Protein Folding

- All-atom and coarse-grained molecular modeling of biophysical systems
- Collective variable discovery and enhanced sampling
- 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
- Data-driven protein engineering

COMMERCIAL INTERESTS

Co-Founder, Evozyne Inc. | www.evozyne.com
- Data-driven protein engineering startup co-founded with Rama Ranganathan

JOURNAL EDITORSHIP

Deputy Editor-in-Chief, *Molecular Systems Design & Engineering* 2023 – present
Topic Editor, *Journal of Physical Chemistry* 2022 – 2023

PROFESSIONAL SOCIETY LEADERSHIP

CECAM-US-CENTRAL Director 2023 – present
- Inaugural director of the first CECAM node in the United States

- Multi-institutional partnership comprising UChicago, Northwestern University, University of Wisconsin-Madison, University of Illinois Urbana-Champaign, University of Notre Dame, and Argonne National Laboratory.

AIChE CoMSEF Chair 2024-26
AIChE CoMSEF Vice Chair 2022-24

- Elected to lead the Computational Molecular Science and Engineering Forum of the American Institute of Chemical Engineers
- Six-year service term (2-years Vice Chair, 2-years Chair, 2-years Chair Emeritus)

AIChE CoMSEF Liaison Director 2016-18, 19

- Facilitate CoMSEF programming and sponsorship, and communicating and advocating activities
- Elected by CoMSEF membership for a 2-year term

AIChE Area 1a Programming Committee 2015-18, 19-21

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

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

25. "Structure and stability of peptoid nanosheets and nanotubes: Computation, experiment, and theory", AIChE Annual Meeting, Orlando, FL, November 6, 2023
24. "Deep learning of low-dimensional latent space molecular simulators" Virtual AIChE Annual Meeting, Nov 15-20 2020
23. "Programming colloidal assembly into aggregates and crystals by landscape engineering" AIChE Annual Meeting, Pittsburgh, PA, Oct 28 – Nov 2 2018
22. "Programmed assembly of anisotropic patchy colloids by nonlinear learning and landscape engineering" AIChE Annual Meeting, Minneapolis, MN, Oct 29 – Nov 3 2017
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

147. "Nano-AI Convergence for Biology and Nanomedicine: Data-driven functional protein design", 2024 NSF Nanoscale Science and Engineering Grantees Conference, Hilton Alexandria Old Town, Washington DC, Dec 10, 2024
146. "Deep generative protein design using natural language text prompts", CECAM Flagship Workshop: Generative models for classical and quantum matter, CECAM-HQ, Lausanne, Switzerland, Dec 4, 2024
145. "Artificial intelligence for biomolecular backmapping and functional protein design", Chemical & Biological Engineering Seminar, Colorado School of Mines, Golden, CO, November 22, 2024
144. "Multi-modal learning for natural language prompt design of novel functional proteins", AIChE Annual Meeting, San Diego, CA, October 29, 2024
143. "Data-driven backmapping of coarse-grained simulations of proteins and DNA", AIChE Annual Meeting, San Diego, CA, October 28, 2024

142. "Data-driven discovery and enhanced sampling in slow collective variables", CECAM Workshop: Expanding the Impact of Molecular Simulations by Integrating Machine Learning with Statistical Mechanics, Grand Hotel Vesuvio, Sorrento, Italy, October 11, 2024
141. "FlowBack: A flow-matching approach for generative backmapping of macromolecules", CECAM Workshop: Leveraging Machine Learning for Sampling Rare Events in Biomolecular Systems, MPI Polymer Research, Mainz, Germany, September 17, 2024
140. "A high-bias, low-variance review of data-driven collective variable discovery and enhanced sampling" + "Molecular latent space simulators: Hands-on tutorial", Learning Collective Variables and Coarse Grained Models, Institute for Mathematical and Statistical Innovation, University of Chicago, Chicago, IL, April 2, 2024
139. "Data-driven protein design and high-fidelity protein backmapping", AI in Science Seminar Series, Schmidt Futures AI in Science Fellowship Program, University of Chicago, Chicago, IL, April 2, 2024
138. "Data-driven protein design using deep generative models", The Automated Scientist, Novo-Nordisk Foundation Science Cluster, Favrholm, Hillerød, Denmark, March 12, 2024
137. "Molecular latent space simulators", JNCASR-CECAM Conference MD@60, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bengaluru 560064, February 29, 2024
136. "DiAMoNDBack: Diffusion-denoising Autogressive Model for Non-Deterministic Backmapping", GNNs for the Sciences, Institute for Mathematical and Statistical Innovation (IMSI), University of Chicago, Chicago, IL, January 25, 2024
135. "DiAMoNDBack: Diffusion-denoising Autogressive Model for Non-Deterministic Backmapping", Machine Learning and Coarse Grained Models Mini-Symposium in Honor of Bernadette Mohr, University of Amsterdam, Amsterdam, Netherlands, December 20, 2023
134. "Data-driven protein design and high-fidelity protein backmapping", Frankfurt Institute for Advanced Studies, Frankfurt, Germany, December 18, 2023
133. "Data-driven protein design and high-fidelity protein backmapping", Chemical Engineering Seminar, Auburn University, Auburn, AL, November 29, 2023
132. "Machine learning-guided directed evolution of functional proteins", AIChE Annual Meeting, Orlando, FL, November 9, 2023
131. "Data-driven protein design and high-fidelity protein backmapping", Physical Chemistry Symposium, Purdue University, West Lafayette, IN, September 27, 2023
130. "Machine learning-guided directed evolution of functional proteins", Chemistry Symposium, Xavier University of Louisiana, New Orleans, LA, September 7, 2023
129. "Machine learning-guided directed evolution of functional proteins", Dreyfus Foundation / ACS Presidential Symposium on Machine Learning, ACS Fall Meeting, San Francisco, CA, August 15, 2023
128. "Tubes or sheets? Prediction and understanding of peptoid supramolecular assembly", Symposium in Celebration of Pablo Debenedetti's 70th Birthday, Princeton University, Princeton, NJ, June 15-17, 2023
127. "DiAMoNDBack: Diffusion-denoising Autogressive Model for Non-Deterministic Backmapping", Machine learning and chemistry: Are we there yet?, NSF MolSSI Workshop, University of Maryland, College Park, MD, May 31 – June 20 2023
126. "Data-driven protein design and ultra-fast molecular simulators", Mathematical Institute Virtual Seminar, University of Oxford, May 5 2023
125. "Machine learning-guided directed evolution of functional proteins", ML4Materials from Molecules to Materials (Virtual), 11th International Conference on Learning Representations, May 4 2023
124. "Machine learning-guided directed evolution of functional proteins", The University of Chicago and Caltech Conference on AI+Science, University of Chicago, Chicago, IL, March 30 2023
123. "Machine learning-guided directed evolution of functional proteins", Molecule Maker Lab Institute, University of Illinois at Urbana-Champaign, Urbana, IL, March 21 2023
122. "Data-driven discovery and enhanced sampling in slow collective variables", Rare Events, Analysis, Numerics, and Applications, Brin Math Research Center, University of Maryland, College Park, MD, February 27 2023
121. "Data-driven protein design and ultra-fast molecular simulators", Lorentz Workshop: Designing Soft Matter in and Out of Equilibrium, Leiden, Netherlands, January 31 2023
120. "Data-driven protein design and ultra-fast molecular simulators", Chemical and Biomolecular Engineering, UC Berkeley, Berkeley, CA, December 7 2022
119. "Data-driven protein discovery", Machine Learning in Materials Discovery, AIChE Annual Meeting, Phoenix, AZ, November 14 2022
118. "Data-driven protein design and ultra-fast molecular simulators", Materials Science and Engineering Seminar, Cornell University, Ithaca, NY, October 27 2022

117. "Molecular latent space simulators", Machine Learning Meets Statistical Mechanics: Success and Future Challenges in Biosimulations, CECAM-IT-SIMUL, Grand Hotel Vesuvio, Sorrento, Italy, October 12-14 2022
116. "Designed by Nature. Engineered by Evozyne.", NVIDIA Healthcare Dev Summit, July 26 2022
115. "Data-driven protein design and ultra-fast molecular simulators", Foundations of Molecular Modeling 2022 (FOMMS 2022), Lake Lawn Resort, Delavan, WI, July 19 2022
114. "Machine learning-enabled enhanced sampling and ultra-fast molecular simulators", ESI-DCAFM-TACO-VDSP Summer School, Erwin Schrödinger Institute, University of Vienna, Vienna, Austria, July 15 2022
113. "A high-bias, low-variance review of data-driven collective variable discovery and enhanced sampling", CECAM Workshop: Chasing CVs using Machine Learning, Inria Paris, Paris, France, June 29 2022
112. "Data-driven protein design and ultra-fast molecular simulators", Computational Soft Matter Seminar, University of Amsterdam, Amsterdam, Netherlands, June 7 2022
111. "Machine learning-enabled enhanced sampling and estimation of folding funnels from experimental data", Amsterdam Center for Multiscale Modelling/John van Geuns Seminar, University of Amsterdam, Amsterdam, Netherlands, June 3 2022
110. "Data-driven protein design and ultra-fast molecular simulators", Institute Seminar, Max Planck Institute for Polymer Research, Mainz, Germany, May 20 2022
109. "Molecular enhanced sampling with autoencoders", CECAM: Machine Learning Augmented Sampling for the Molecular Sciences, CECAM-HQ, Lausanne, Switzerland, May 10 2022
108. "Data-driven design of self-assembling optoelectronic peptides", Workshop on Data-Driven Design of Heterogeneous Materials, University of Chicago, May 6 2022
107. "Data-driven protein design and ultra-fast molecular simulators", Chemistry Symposium, Iowa State University, Ames, IA, April 29 2022
106. "Data-driven protein design", NSF NRT Symposium, University of Delaware, April 22 2022
105. "Data-driven protein design", OneChemistry Symposium, Johns Hopkins University, Baltimore, MD, April 19 2022
104. "Data-driven protein design and ultra-fast molecular simulators", Chemistry Seminar, Carnegie Mellon University, April 8 2022
103. "Data-driven protein design and ultra-fast molecular simulators", Chemical Engineering Seminar, UC Santa Barbara, Santa Barbara, CA, April 4 2022
102. "AI-accelerated Molecular Dynamics and Protein Engineering for Drug Discovery", Panelists: Juan Carlos Mobarec (AstraZeneca), Mark Moraes (DE Shaw Research), Huafeng Xu (Roivant Discovery), Andrew Ferguson (Evozyne/UChicago), Virginia Burger (New Equilibrium Biosciences), Andrew Ban (Arzeda), NVIDIA GTC, March 23 2022
101. "Data-driven protein design", Statistical Thermodynamics and Molecular Simulations (STMS) Seminar Series (https://sites.google.com/view/stms2021), March 18 2022
100. "Data-driven molecular simulators for biomolecular folding", Recent Developments in Computer Simulational Studies in Condensed Matter Physics Center for Simulational Physics, University of Georgia, Feb 24 2022
99. "Data-driven protein design and ultra-fast molecular simulators", Chemical Engineering Seminar, Oklahoma State University, Jan 25 2022
98. "Ultra-fast molecular simulators and data-driven protein design", AI4Science Colloquium, AI4Science Lab, University of Amsterdam, Jan 18 2022
97. "Molecular latent space simulators for molecular degrader design", Recent Advances in Modelling Rare Events (RARE2021), Dec 15-18 2021
96. "Ultra-fast molecular simulators and data-driven protein design", Chemical Engineering Seminar, UIC, Chicago, IL, Dec 2 2021
95. "Data-driven protein engineering using deep representational active learning", Special Session In Honor of Arup Chakraborty's 60th Birthday: Statistical Mechanics and Molecular/Materials Modeling, AIChE Annual Meeting, Boston, MA, Nov 9 2021
94. "Data-driven protein design and simulation", Division of Chemical and Polymer Physics (CPP) – CPP 15: Theory and Simulation, German Physical Society (DPG) Meeting, September 27 - October 1 2021
93. "Molecular latent space simulators", Accelerating the Understanding of Rare Events, Lorentz Center at Oort, September 6-10 2021
92. "Deep learning in protein folding: Trajectory reconstruction from experimental measurements and data-driven protein design", Virtual Computational Chemistry Seminar, University of Strathclyde, June 29 2021

91. "Deep learning in protein folding: Trajectory reconstruction from experimental data and ultra-fast latent space simulators", Virtual Chemistry Seminar, HKUST, June 2 2021
90. "Machine learning-enabled high-throughput virtual screening for novel mitochondrial membrane dyes", Virtual MRS Spring Meeting, April 20 2021
89. "Data science in soft materials engineering: Enhanced sampling and data-driven molecular design" & "Deep learning in protein folding: Trajectory reconstruction and ultra-fast simulators", Virtual Theoretical Chemistry Lecture Series, Boston University, Boston, MA, March 31 2021
88. "Molecular Latent Space Simulators", Predicting Rare Event Kinetics in Complex Systems with Theory, Simulations and Machine Learning I, Virtual APS March Meeting, March 15-19 2021
87. "Deep learning in protein folding: Trajectory reconstruction and ultra-fast simulators", Bioengineering Subgroup Symposium, Virtual 65th Biophysical Society Annual Meeting, Feb 22-26 2021
86. "Reconstructing protein folding trajectories from experimentally measurable observables", Machine Learning in Science & Engineering Virtual Meeting, The Data Science Institute, Columbia University, New York, NY, Dec 14 2020
85. "Molecular latent space simulators", 2020 Virtual MRS Spring/Fall Meeting, Dec 2 2020
84. "Molecular latent space simulators", Virtual Integrated Applied Math Seminar, University of New Hampshire, Oct 29 2020
83. "Dynamical coarse graining: Trajectory reconstruction and molecular latent space simulators", CECAM Virtual Flagship Workshop: Multiscale simulations of soft matter: New method developments and mathematical foundations, CECAM-DE-SMSM Digital Event, Sep 30 - Oct 2 2020
82. "Coarse graining in time: Latent space simulators", CECAM Flagship Workshop: (Machine) Learning How to Coarse Grain, CECAM-DE-SMSM Digital Event, Sep 28-29 2020
81. "Deep learning in protein folding: Trajectory reconstruction and ultra-fast simulators", Statistical Physics Seminar, University of Maryland, College Park, MD, Sep 22 2020
80. "Deep learning in protein folding: Trajectory reconstruction and ultra-fast simulators", Department of Chemical Engineering, MIT, Cambridge, MA, Sep 18 2020
79. "Reconstructing all-atom protein folding from low-dimensional experimental time series", FAIR-DI e.V. Virtual Conference on a FAIR Data Infrastructure for Materials Genomics, Jun 3-5 2020 [https://youtu.be/3IGv5m8QRJ8]
78. "Reconstructing all-atom protein folding funnels from low-dimensional experimental time series", Department of Physics, UW Milwaukee, Milwaukee, WI, Jan 31 2020
77. "Deep learning of slow collective variables to understand and accelerate biomolecular folding and assembly", New Frontiers of Molecular Thermodynamics (Invited Talks), AIChE Annual Meeting, Orlando, FL, Nov 14 2019
76. "Deep learning of low-dimensional latent space molecular simulators", In Honor of Yannis Kevrekidis' 60th Birthday (Invited Talks), AIChE Annual Meeting, Orlando, FL, Nov 12 2019
75. "Data-driven design of self-assembling pi-conjugated oligopeptides (Invited Talk)", Data-Driven Design and Modeling of Biomaterials, AIChE Annual Meeting, Orlando, FL, Nov 12 2019
74. "Data-driven design of self-assembling optoelectonic π-conjugated oligopeptides and latent space molecular simulators", Department of Chemical and Biomolecular Engineering, UCLA, Los Angeles, CA, October 25 2019
73. "Machine learning of protein folding funnels from experimental data and construction of latent space molecular simulators", Machine Learning for Physics and the Physics of Learning – Workshop II: Interpretable Learning in Physical Sciences, Institute for Pure and Applied Mathematics, UCLA, Los Angeles, CA, October 18 2019
72. "Data-driven design of self-assembling optoelectonic π-conjugated oligopeptides and latent space molecular simulators", Department of Chemical and Biological Engineering, UC Boulder, Boulder, CO, October 1 2019
71. "Machine learning and data science in soft materials design and engineering", Machine Learning for Physics and the Physics of Learning – Long Program Tutorial, Institute for Pure and Applied Mathematics, UCLA, Los Angeles, CA, September 9 2019
70. "Data-driven design of self-assembling optoelectronic π-conjugated oligopeptides and latent space molecular simulators", Physical Science and Engineering AI Seminar, Argonne National Laboratory, Argonne, IL, August 15 2019
69. "Learning of slow dynamical variables to understand and accelerate biomolecular folding", CECAM Workshop: Learning the Collective Variables of Biomolecular Processes, INRIA, Paris, France, July 10 2019
68. "Data-driven design of self-assembling photonic crystals and machine learning of latent space molecular simulators", Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL, June 26 2019
67. "Learning variables for understanding and design of colloidal assembly and protein folding", Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM, June 17 2019

66. "State-free reversible VAMPnet learning of collective variables to understand and accelerate biomolecular folding", SIAM Conference on Applications of Dynamical Systems (DS19): MS164 Theory and Application of Koopman Operator Methods in Molecular Simulation, Snowbird, UT, May 23 2019
65. "Deep learning of collective variables to understand and accelerate biomolecular folding" Topics in Molecular Science and Engineering Symposium, Institute for Molecular Science and Engineering, Imperial College London, London, UK, May 13 2019
    → Presentation of the Institution of Chemical Engineers 2018/19 Junior Moulton Medal for best paper published by the Institution from an author within 10 years of their PhD: A.W. Long and A.L. Ferguson "Rational design of patchy colloids via landscape engineering" *Mol. Syst. Des. Eng.* 3 1 49-65 (2018) [http://dx.doi.org/10.1039/C7ME00077D]
64. "Learning collective variables for understanding and design of colloidal assembly and protein folding" Molecular Sciences Software Institute (MolSSI) and Department of Chemistry, Virginia Tech, Blacksburg, VA, May 3 2019
63. "Learning collective variables for understanding and design of colloidal assembly and protein folding" Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, MD, April 10 2019
62. "Deep learning to understand and accelerate molecular simulations of protein folding" National Academy of Engineering / Alexander von Humboldt Foundation 18th German-American Frontiers of Engineering (FOE) Symposium, Hamburg, Germany, Mar 20 2019 [Poster]
61. "Data-driven learning of collective variables to understand and accelerate biomolecular folding" APS March Meeting: Session A51 Big Data, Polymers, and Soft Matter: New Developments in Machine Learning, Data Mining and High-Throughput Studies, Boston, MA, Mar 4 2019
60. "Artificial Intelligence in Chemical and Materials Science" Chicagoland AI + Science Initiative (University of Chicago, Argonne National Laboratory, Fermi National Accelerator Laboratory, Toyota Technological Institute at Chicago), U. Chicago Plenary Speaker, University of Chicago, Chicago, IL, Jan 25 2019
59. "Machine learning and data science for understanding and design in colloidal assembly and protein folding", Materials Technology Center / Department of Chemistry and Colloquium, Southern Illinois University, Carbondale, IL, Jan 18 2019
58. "Machine learning collective variable discovery in colloidal assembly and protein folding" James Franck Institute Seminar, University of Chicago, Chicago, IL, Jan 8 2019
57. "Enhanced sampling in data-driven collective variables in protein folding and colloid design" Lorentz Center @ Oort Workshop: Machine Learning and Reverse Engineering for Soft Materials, Leiden, Netherlands, Dec 11 2018
56. "Machine learning collective variable discovery in colloidal assembly and protein folding" CECAM discussion meeting: Coarse-graining with machine learning in molecular dynamics, CERMICS, Ecole des Ponts ParisTech, Paris, France, Dec 4 2018
55. "Teaching machines to engineer colloidal crystals and learn protein folding funnels" Department of Chemical and Biomolecular Engineering Seminar, Tulane University, New Orleans, LA, Oct 9 2018
54. "Machine learning design of self-assembling colloidal crystals and inference of protein folding funnels" Department of Chemical and Biological Engineering Seminar, University of Wisconsin, Madison, WI, Oct 2 2018
53. "Machine learning inverse design of self-assembling colloidal assemblies" Frontiers of Molecular Engineering Symposium, University of Chicago, Chicago, IL, Sep 27-28 2018
52. "Data-driven design of self-assembling colloids and machine learning of protein folding funnels" Chemical and Biomolecular Engineering Seminar, Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA, Sep 12 2018
51. "Machine learning collective variable discovery for materials design and engineering" CICS Seminar, Center for Informatics and Computational Science, University of Notre Dame, Notre Dame, IN, Sep 5 2018
50. "Machine learning collective variable discovery for materials design and engineering" D2. Machine Learning and Data Science in Materials Synthesis, Characterization and Modeling, XXVII International Materials Research Congress, Sociedad Mexicana de Materiales/Materials Research Society (MRS), Cancun, Mexico, Aug 19-24 2018
49. "Molecular enhanced sampling with autoencoders: On-the-fly nonlinear collective variable discovery and accelerated molecular free energy landscape exploration" New Developments in Hierarchical Structure and Dynamics of Polymers, GRC Polymer Physics, Mount Holyoke College, South Hadley, MA, July 22-27 2018
48. "Nonlinear machine learning in soft materials engineering and design" MS94 Machine Learning for Predictive Atomistic Simulation of Materials, SIAM Annual Meeting, Portland, OR, July 9-13 2018
47. "Machine learning collective variable discovery for materials design and engineering" AIChE Spring Meeting, Orlando, FL, April 22-26 2018
46. "Machine learning inference and engineering of colloidal self-assembly and macromolecular folding" Chemistry Seminar, Department of Chemistry, University of Vermont, Burlington, VT, April 2 2018

45. "Inference and exploration of macromolecular folding funnels using manifold and deep learning" Chemistry Seminar, Department of Chemistry, University of North Dakota, Grand Forks, ND, February 23 2018
44. "Programmed assembly of anisotropic patchy colloids by landscape engineering" Data-driven Discovery and Design in Soft and Biological Materials, Aspen Center for Physics 2018 Winter Conference, Aspen Center for Physics, Aspen, CO, January 7-13 2018
43. "Molecular enhanced sampling with autoencoders: On-the-fly nonlinear collective variable discovery and accelerated free energy landscape exploration" Recent Advances in Modeling Rare Events (RARE): Methods and Applications, Jaypee Palace Hotel, Agra, India, December 7-10 2017
42. "Statistical learning of viral fitness landscapes" Physical Concepts and Computational Models in Immunology, MIT, Cambridge, MA, October 11-12 2017
41. "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
40. "Machine learning in soft and biological materials: Engineering self-assembling colloids and viral phase behavior" Department of Materials Science and Engineering, UIUC, Urbana, IL, September 18 2017
39. "Machine learning in soft and biological materials: Engineering self-assembling colloids and viral phase behavior" 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

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6. N. Praljak, H. Yeh, M. Moore, M. Socolich, R. Ranganathan, and **A.L. Ferguson** "Natural language prompts guide the design of novel functional protein sequences" NeurIPS 2024 Workshop AIDrugX, Vancouver, CA, December 15, 2024 [https://openreview.net/forum?id=L1MyyRCAjX&noteId=L1MyyRCAjX]
5. M. Jones, S. Khanna, and **A.L. Ferguson** "FlowBack: A Flow-matching Approach for Generative Backmapping of Macromolecules" ICML'24 Workshop ML for Life and Material Science (ML4LMS): From Theory to Industry Applications, Vienna, Austria, July 26, 2024 [https://openreview.net/forum?id=mhUasr0j5X]
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3. X. Zhang, A. Schleife, **A.L. Ferguson**, P. Bellon, T. Bretl, G.L. Herman, J.A. Krogstad, C.R. Maass, C. Leal, D.R. Trinkle, and M. West "Computational Curriculum for MatSE Undergraduates and the Influence on Senior Classes" Paper presented at 2018 American Society for Engineering Education (ASEE) 125th Annual Conference & Exposition, Salt Lake City, UT, June 24-27 2018 [https://peer.asee.org/30213]
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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** "Chapter 17: 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 pp. 279-298 (2019) [ISBN-10: 1498717403]

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2. "Community Values, Guiding Principles, and Commitments for the Responsible Development of AI for Protein Design" (March 8, 2024) [https://responsiblebiodesign.ai/]
1. **A.L. Ferguson**, Benoît Roux, John S. Anderson, Adam T. Hammond, Graham J. Slater, Henry Hoffmann, and Aaron P. Esser-Kahn "In Defense of DEI in Science" The Chicago Maroon (Oct 12, 2023) [https://chicagomaroon.com/39973/viewpoints/op-ed/in-defense-of-dei-in-science/]

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* *Designates corresponding author.*

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80. Y. Xia, Z. Song, T. Xue, S. Wei, L. Zhu, Z. Tan, Y. Yang, H. Fu, Y. Jiang, Y. Lin, Y. Lu, **A.L. Ferguson***, and J. Cheng "Accelerated polymerization of N-carboxyanhydrides catalyzed by crown ether" *Nat. Commun.* 12 732 (2021) [https://doi.org/10.1038/s41467-020-20724-w]
→ Selected for Editors' Highlight of 50 best recent papers published in organic chemistry and chemical biology

79. C.H. Fry, B. Peters, and **A.L. Ferguson** "Pushing and pulling: A dual pH triggered heme peptide assembly" *J. Phys. Chem. B* 125 5 1317-1330 (2021) [https://dx.doi.org/10.1021/acs.jpcb.0c07713]

78. E.Y. Lee, L.C. Chan, H. Wang, J. Lieng, M. Hung, Y. Srinivasan, J. Wang, J. Waschek, **A.L. Ferguson**, K.-F. Lee, N.Y. Yount, M.R. Yeaman, and G.C.L. Wong "Mood-modulating neuropeptide PACAP is potently induced during infection" *Proc. Natl. Acad. Sci. USA* 118 1 e1917623117 (2020) [https://doi.org/10.1073/pnas.1917623117]
→ Highlighted in an accompanying commentary article: M. Zasloff "An ancient neuropeptide defends the brain against infection" *PNAS* 118 5 e2023990118 (2020)

77. **A.L. Ferguson***, J. Hachmann, T.F. Miller, and J. Pfaendtner "Editorial: The Journal of Physical Chemistry A/B/C Virtual Special Issue on Machine Learning in Physical Chemistry" *J. Phys. Chem B* 124 9767–9772 (2020) [https://dx.doi.org/10.1021/acs.jpcb.0c09206]
→ Invited editorial for the "Virtual Special Issue on Machine Learning in Physical Chemistry"

76. B. Sharma, Y. Ma, **A.L. Ferguson***, and A.P. Liu "In search of a novel chassis material for synthetic cells: Emergence of synthetic peptide compartment" *Soft Matter* 16 10769 (2020) [https://dx.doi.org/10.1039/D0SM01644F]

75. M. Topel and **A.L. Ferguson*** "Reconstruction of protein structures from single molecule time series" *J. Chem. Phys.* 153 194102 (2020) [https://doi.org/10.1063/5.0024732]
→ Invited submission to the "2020 JCP Emerging Investigators in Science Collection"

74. H. Sidky, W. Chen, and **A.L. Ferguson*** "Molecular latent space simulators" *Chem. Sci.* 11 9459 (2020) [http://dx.doi.org/10.1039/D0SC03635H]
→ Selected for 2020 Chemical Science HOT Article Collection

73. M. Zhao, J. Sampath, S. Alamdari, G. Shen, C.-L. Chen, C.J. Mundy, J. Pfaendtner, and **A.L. Ferguson*** "MARTINI-compatible coarse-grained model for the mesoscale simulation of peptoids" *J. Phys. Chem. B* 124 36 7745–7764 (2020) [http://dx.doi.org/10.1021/acs.jpcb.0c04567]

72. P. Gkeka, G. Stoltz, A. Barati Farimani, Z. Belkacemi, M. Ceriotti, J. Chodera, A. Dinner, **A.L. Ferguson**, J.-B. Maillet, H. Minoux, C. Peter, F. Pietrucci, A. Silveira, A. Tkatchenko, Z. Trstanova, R. Wiewiora, and T. Lelievre "Machine learning force fields and coarse-grained variables in molecular dynamics: Application to materials and biological systems" *J. Chem. Theory Comput.* 16 8 4757–4775 (2020) [https://doi.org/10.1021/acs.jctc.0c00355]

71. S. Panda, K. Shmilovich, **A.L. Ferguson**, and J.D. Tovar "Computationally guided tuning of amino acid configuration influences the chiroptical properties of supramolecular peptide-π-peptide nanostructures" *Langmuir* 36 24 6782–6792 (2020) [https://dx.doi.org/10.1021/acs.langmuir.0c00961]

70. B.L. Peters, J. Deng, and **A.L. Ferguson*** "Free-energy calculations of the functional selectivity of 5-HT_{2B} G protein coupled receptor" *PLoS ONE* 15 12 e0243313 (2020) [https://doi.org/10.1371/journal.pone.0243313]

69. E. Jira, K. Shmilovich, T. Kale, **A.L. Ferguson**, J.D. Tovar, and C. Schroeder "Effect of core oligomer length on the phase behavior and assembly of π-conjugated peptides" *ACS Appl. Mater. Interfaces* 12 20722-20732 (2020) [https://dx.doi.org/10.1021/acsami.0c02095]

68. K. Shmilovich, R.A. Mansbach, H. Sidky, O.E. Dunne, S.S. Panda, J.D. Tovar, and **A.L. Ferguson*** "Discovery of self-assembling π-conjugated peptides by active learning-directed coarse-grained molecular simulation" *J. Phys. Chem. B* 124 3873-3891 (2020) [https://doi.org/10.1021/acs.jpcb.0c00708]
→ Invited submission to the "Machine Learning in Physical Chemistry" special issue
→ Selected as ACS Editors' Choice article (March 30, 2020)
→ Selected for front cover art of JPCB vol. 124, issue 19 (May 14, 2020)

67. M.R. Shirts and **A.L. Ferguson*** "Statistically optimal continuous potentials of mean force from umbrella sampling and multistate reweighting" *J. Chem. Theory Comput.* 16 7 4107–4125 (2020) [https://dx.doi.org/10.1021/acs.jctc.0c00077]

66. H. Sidky, W. Chen, and **A.L. Ferguson*** "Machine learning for collective variable discovery and enhanced sampling in biomolecular simulation" *Molecular Physics* 118 5 e1737742 (2020) [https://doi.org/10.1080/00268976.2020.1737742]
→ Invited New Views article in *Molecular Physics*

65. M. Magana, M. Pushpanathan, A. Santos, L. Lense, M. Fernandez, A. Ioannidis, M.A. Giulianotti, Y. Apidianakis, S. Bradfute, **A.L. Ferguson**, A. Cherkasov, M.N. Seleem, C. Pinilla, C. de la Fuente-Nunez, T. Lazaridis, T. Dai, R.A. Houghten, R.E.W. Hancock, and G.P. Tegos "The value of antimicrobial peptides in the age of resistance" *The Lancet Infectious Diseases* (2020) [https://doi.org/10.1016/S1473-3099(20)30327-3]

64. B.A. Thurston, E.P. Shapera, J.D. Tovar, A. Schleife, and **A.L. Ferguson*** "Revealing the sequence-structure-electronic property relation of self-assembling π-conjugated oligopeptides by molecular and quantum mechanical modeling" *Langmuir* 35 47 15221-15231 (2019) [https://doi.org/10.1021/acs.langmuir.9b02593]

63. S. Panda, K. Shmilovich, **A.L. Ferguson***, and J.D. Tovar "Controlling supramolecular chirality in peptide-π-peptide networks by variation of alkyl spacer length" *Langmuir* 35 43 14060-14073 (2019) [https://doi.org/10.1021/acs.langmuir.9b02683]
62. The PLUMED Consortium (M. Bonomi, G. Bussi, C. Camilloni, G.A. Tribello, P. Banáš, A. Barducci, M. Bernetti, P.G. Bolhuis, S. Bottaro, D. Branduardi, R. Capelli, P. Carloni, M. Ceriotti, A. Cesari, H. Chen, W. Chen, F. Colizzi, S. De, M. De La Pierre, D. Donadio, V. Drobot, B. Ensing, **A.L. Ferguson**, M. Filizola, J.S. Fraser, H. Fu, P. Gasparotto, F. Luigi Gervasio, F. Giberti, A. Gil-Ley, T. Giorgino, G.T. Heller, G.M. Hocky, M. Iannuzzi, M. Invernizzi, K.E. Jelfs, A. Jussupow, E. Kirilin, A. Laio, V. Limongelli, K. Lindorff-Larsen, T. Löhr, F. Marinelli, L. Martin-Samos, M. Masetti, R. Meyer, A. Michaelides, C. Molteni, T. Morishita, M. Nava, C. Paissoni, E. Papaleo, M. Parrinello, J. Pfaendtner, P. Piaggi, G. Piccini, A. Pietropaolo, F. Pietrucci, S. Pipolo, D. Provasi, D. Quigley, P. Raiteri, S. Raniolo, J. Rydzewski, M. Salvalaglio, G. Cesare Sosso, V. Spiwok, J. Šponer, D.W.H. Swenson, P. Tiwary, O. Valsson, M. Vendruscolo, G.A. Voth, and A. White) "A community effort to promote transparency and reproducibility in enhanced molecular simulations" *Nat. Methods* 16 8 670-673 (2019) [https://doi.org/10.1038/s41592-019-0506-8]
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58. **A.L. Ferguson***, T. Mueller, S. Rajasekaran, and B.J. Reich "Conference report: 2018 materials and data science hackathon (MATDAT18)" *Mol. Syst. Des. Eng.* 4 462-468 (2019) [https://doi.org/10.1039/c9me90018g]
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55. Z. Song, H. Fu, J. Wang, J. Hui, T. Xue, L.A. Pacheco, H. Yan, R. Baumgartner, Z. Wang, Y. Xia, X. Wang, L. Yin, C. Chen, J. Rodríguez-López, **A.L. Ferguson**, Y. Lin, and J. Cheng "Synthesis of polypeptides via bio inspired polymerization of in situ purified N-carboxyanhydrides" *Proc. Natl. Acad. Sci. USA* 116 22 10658-10663 (2019) [https://doi.org/10.1073/pnas.1901442116]
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53. M.W. Lee, E.Y. Lee, **A.L. Ferguson**, and G.C.L. Wong "Machine learning antimicrobial peptide sequences: Some surprising variations on the theme of amphiphilic assembly" *Curr. Opin. Colloid Interface Sci.* 38 204-213 (2018) [https://doi.org/10.1016/j.cocis.2018.11.003]
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51. **A.L. Ferguson*** "Editorial: ACS Central Science Virtual Issue on Machine Learning" *ACS Cent. Sci.* 4 8 938-941 (2018) [http://dx.doi.org/10.1021/acscentsci.8b00528]
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50. G.R. Hart and **A.L. Ferguson*** "Computational design of hepatitis C virus immunogens from host-pathogen dynamics over empirical viral fitness landscapes" *Physical Biology* 16 016004 (2018) [https://doi.org/10.1088/1478-3975/aaeec0]
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    → Top 10% or most downloaded papers in 12 months following online publication for period Jan 2018 - Dec 2019
42. **A.L. Ferguson*** and J. Hachmann "Machine learning and data science in materials design: a themed collection" *Mol. Syst. Des. Eng.* 3 429-430 (2018) [https://doi.org/10.1039/C8ME90007H]
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41. 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* 51 2 598-616 (2018) [http://dx.doi.org/10.1021/acs.macromol.7b01684]
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39. A.W. Long and **A.L. Ferguson*** "Rational design of patchy colloids via landscape engineering" *Mol. Syst. Des. Eng.* 3 1 49-65 (2018) [http://dx.doi.org/10.1039/C7ME00077D]
    → Invited submission to the 2018 Emerging Investigators issue
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    → Selected by journal as winner of RSC MSDE Emerging Investigator Award
    → Awarded the Institution of Chemical Engineers 2018/19 Junior Moulton Medal for best paper published by the Institution from an author within 10 years of their PhD
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37. **A.L. Ferguson*** "Machine learning and data science in soft materials engineering" *J. Phys.: Condens. Matter* 30 4 043002 (2017) [http://dx.doi.org/10.1088/1361-648X/aa98bd]
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36. 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.* 3 11 1156-1167 (2017) [http://dx.doi.org/10.1021/acscentsci.7b00338]
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35. 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* 7 20160153 (2017) [http://dx.doi.org/10.1098/rsfs.2016.0153]
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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]
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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]
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   → Editorial selection as feature in Cell "Select" series on antiviral strategies in *Cell* 153 4 (2013)
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   → Featured as the cover article of Journal of Chemical Physics 137 (2012)
   → Most read regular Journal of Chemical Physics article in October 2012
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   → 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]

PATENTS

5. Title: INNATE IMMUNOMODULATORS
   Filing Date: June 16, 2023
   Inventors: Andrew L. Ferguson, Aaron Esser-Kahn
   U.S. Provisional Patent Application No.: 63/521,617
4. Title: ARTIFICIAL INTELLIGENCE (AI)-BASED PROTEIN ENGINEERING SYSTEMS AND METHODS FOR DESIGNING SYNTHETIC PROTEIN SEQUENCES
   Filing Date: January 11, 2023
   Inventors: Andrew L. Ferguson, Emre Sevgen, Joshua Moller, Adrian Lange
   U.S. Provisional Patent Application No.: 63/479,378
3. Title: DATA-DRIVEN PROTEIN DESIGN USING NORMALIZING FLOWS AND LATENT-CONDITIONED DILATED CASUAL CONVOLUTIONS

Filing Date: February 28, 2022
Inventors: Nikša Praljak, Andrew L. Ferguson
U.S. Provisional Patent Application No.: 63/314,898

2. Title: METHOD AND APPARATUS USING MACHINE LEARNING FOR EVOLUTIONARY DATA-DRIVEN DESIGN OF PROTEINS AND OTHER SEQUENCE DEFINED BIOMOLECULES
Filing Date: September 13, 2019
Inventors: Rama Ranganathan, Andrew L. Ferguson
U.S. Provisional Patent Application No.: 62/900,420
U.S. Patent Application No.: 17/642,582
International Patent Application No.: PCT/US2020/050466

1. Title: HIV-1 SPECIFIC IMMUNOGEN COMPOSITIONS AND METHODS OF USE
Filing Date: May 29, 2019
Inventors: Darrell J. Irvine, Daniel H. Barouch, Arup K. Chakraborty, Dariusz Murakowski, Bruce D. Walker, John Barton, Andrew L. Ferguson
U.S. Provisional Patent Application No.: 62/853,919
U.S. Patent Application No.: 16/887,710
International Patent Application No.: PCT/US2020/035206

TEACHING

MENG 24300 –Molecular Modeling U. Chicago 2023, 24
Theory and practice of quantum and classical molecular modeling prioritizing hands-on project-based learning

MENG 25500/35500 – Classical Molecular and Materials Modeling U. Chicago 2019, 20, 21, 23, 24
Theory and practice of classical molecular modeling focusing on Monte-Carlo and molecular dynamics

MENG 23100 – Applied Numerical Methods in Molecular Eng. U. Chicago 2019
Training in the theory and hands-on practice of numerical tools to solve problems in molecular engineering

ENG 198 – Grand Challenges UIUC 2012-14
Freshman enrichment elective guiding teams in the study of one of the NAE Grand Challenges

MSE 458 – Polymer Physics UIUC 2013-18
Intermediate-level introduction to the equilibrium physics and physical chemistry of polymer systems

MSE 498 – Computational Materials Science and Engineering UIUC 2013-15
MSE 404 – Computational Materials Science and Engineering UIUC 2016-17
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 (International)

Recent Advances in Modelling Rare Events (RARE2025) Khajuraho, India
- Co-organizer with Nisanth N. Nair (IIT Kanpur), Jagannath Mondal (TIFR Hyderabad), Suman Chakrabarty (SNBNCBS, Kolkata), Tarak Karmakar (IIT Delhi) March 9-12 2025
- Indo-US bilateral workshop focused on novel computational methods for rare event sampling and machine learning

Recent Advances in Modelling Rare Events (RARE2021) Virtual
- Co-organizer with Amalendu Chandra (IIT Kanpur), Pratyush Tiwary (U Maryland) Jagannath Mondal (TIFR Hyderabad), and Nisanth N. Nair (IIT Kanpur) December 15-18 2021
- Indo-US bilateral workshop focused on novel computational methods for rare event sampling and machine learning

Lorentz Center @ Oort Workshop: Leiden, Netherlands
Machine Learning and Reverse Engineering for Soft Materials December 10-14 2018
- Co-organizer with Erik Luijten (MSE, Northwestern) and Marjolein Dijkstra (Debye Institute, Utrecht)
- Workshop on porting of data science and informatics tools to soft materials science, engineering, and design
- Bringing together participants in soft materials and informatics for talks, discussion, and mini-hackathon

Conference Organization (National)

FOMMS 2024 Programming Chair Snowbird, UT

- Programming co-organizer of 2024 Foundations of Molecular Modeling and Simulation July 28 – Aug 1 2024

IMSI Workshop Organizer Chicago, IL
- Co-organizer of workshop "Learning Collective Variables and Coarse Grained Models" April 22-26 2024
  At the Institute for Mathematical and Statistical Innovation center at UChicago

AIChE Annual Meeting 2023 Session Organizer Orlando, FL
CoMSEF Poster Session Nov 5-10 2023

Workshop on Data-Driven Design of Heterogeneous Materials Chicago, IL
- Co-organizer with Juan de Pablo and supported by the Army Research Office Materials Design Program led by Dr. Evan Runnerstrom May 5-6 2022
- Two-day workshop bringing together data scientists and materials scientists to identify pressing challenges and priorities in the data-driven design of soft, hard and heterogeneous materials and define potential paths forward.

AIChE Annual Meeting 2021 Session Organizer Boston, MA
Applications of Data Science in Molecular Sciences I & II Nov 7-9 2021
Special Session In Honor of Arup Chakraborty's 60th Birthday [Invited Talks]

APS March Meeting 2021 Session Chair Virtual
P25: Predicting Rare Event Kinetics in Complex Systems II March 15-19 2021

AIChE Annual Meeting 2020 Session Organizer San Francisco, CA
Applications of Data Science in Molecular Sciences I & II Nov 15-20 2020

Workshop on Data-Driven Design of Heterogeneous Materials @ UChicago Aug 31 – Sep 1 2020
- Co-organizer with Juan de Pablo and supported by the Army Research Office Materials Design Program led by Dr. Evan Runnerstrom
- One-day virtual workshop bringing together data scientists and materials scientists to identify pressing challenges and priorities in the data-driven design of soft, hard and heterogeneous materials and define potential paths forward.

Experiences of Black STEM in the Ivory: A Call to Disruptive Action July 14-15 2020
- Co-organizer with colleagues from UW Seattle, Georgia Tech, UT Austin, and Boston University
- Two-day virtual event hosting students, staff, faculty and leadership panels discussing barriers facing Black scholars in STEM and the goal of catalyzing concrete and meaningful action

AIChE Annual Meeting 2019 Session Organizer Orlando, FL
Applications of Data Science in Molecular Sciences I & II Nov 10-15 2019
CoMSEF Poster Session

AIChE Annual Meeting 2018 Session Organizer Pittsburgh, PA
In Honor of Pablo Debenedetti II (Invited Talks) Oct 28 – Nov 2 2018
Data Mining and Machine Learning in Molecular Sciences I & II

MATDAT18: Materials and Data Science Hackathon Alexandria, VA
- Co-organizer with Tim Mueller (MSE, JHU), Sanguthevar Rajasekaran (CSE, UConn), and Brian Reich (Stats, NCSU) May 30 – June 1 2018
- NSF-funded "hackathon" bringing materials ("mat") and data ("dat") scientists together to spark collaborations and apply advanced data science methods to address challenging problems in materials science and engineering

APS GSOFT Short Course: Machine Learning and Data Science in Soft Matter Los Angeles, CA
- Co-organizer with Eric Jankowski (MSE, Boise State) March 4 2018
- One-day workshop on data science and machine learning tools in soft materials
- Tutorial-style lectures from leading practitioners in the field and a hands-on Python workshop

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

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

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

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

Conference Organization (Regional)

Scottish Chemistry Burns Symposium — U. Chicago
Co-organizer w/ Stuart Rowan — January 25 2019

- Symposium of Scottish chemists honoring the birth of Scottish poet Robert Burns
- Keynote speaker Sir J. Fraser Stoddart, 2016 Nobel Laureate in Chemistry

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

Scientific Advisory Boards

Department of Chemical Engineering, Imperial College London — 2023 – present

Journal Advisory Boards

Journal of Physical Chemistry (ACS) — 2020 – 2022
Molecular Systems Design and Engineering (RSC, IChemE) — 2017 – 2018

Journal Editorial Boards

Molecular Systems Design and Engineering (RSC, IChemE) — 2018 – 2024

Professional Consortia

PLUMED Consortium (https://www.plumed-nest.org/consortium.html) — 2019 – present

Mentorship and Outreach

PME-City Colleges of Chicago Summer Program — U. Chicago
Instructor — Summer 2020, 2021

- Developed and delivered computational molecular engineering course materials to City Colleges of Chicago students

PME's After School Matters Program — U. Chicago
Mentor — Summer 2019

- Supported two high school student summer researchers in performing college-level research

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 – Spring 2017

- 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

Workshop Participation

Camille and Henry Dreyfus Foundation: Machine Learning for the Chemical Sciences and Engineering — New York City
Participant — April 26 2019

- Invited meeting attendee and participant

National Academy of Engineering / Alexander von Humboldt German-American Frontiers of Engineering Symposium Invited Participant — Hamburg, Germany
Moderator and Panelist — March 20-23 2019

- Invited workshop participant and poster presenter in thematic area Artificial Intelligence and Deep Learning

National Academies Chemical Sciences Roundtable: Data Science: Opportunities to Transform Chemical Sciences and Engineering — NAS Building, D.C.
Moderator and Panelist — February 27-28 2018

- Invited speaker, panelist, and participant in workshop on data science in the chemical sciences
https://nas-sites.org/csr/data-science-opportunities-to-transform-chemical-sciences-engineering/
https://vimeo.com/album/5090055/video/262998664

National Academies Chemical Sciences Roundtable Business Meeting — Nat'l Acad. Keck Center
Moderator and Panelist — July 20 2017

- Speaker and participant in session "Data Science in Chemistry and Chemical Engineering"
- Workshop and discussion to determine directions and topics of future NAS CSR workshops

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

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

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

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

Department and Campus Service

Future of Research Computing Infrastructure Committee — U. Chicago
Committee Member — 2024

- Committee member assembling report and recommendations to Provost and President on the future of research computing infrastructure at UChicago

University of Chicago Campus Climate Survey Advisory Committee — U. Chicago
Committee Member and PME Representative — 2023

- PME faculty representative in design of 2023 Campus Climate Survey

New Engineering and Science Building (NESB) Planning Committee — U. Chicago
Committee Member and Theory Lead — 2022-present

- Faculty representative in planning for new building design

Biological Engineering Planning Committee — U. Chicago
Committee Member — 2022-present

- Envisioning and planning for new Biological Engineering Department

Physical Sciences Division EDI Coordination Team — U. Chicago
Committee Member and PME Liaison — 2021-22

- Faculty advocate, leader, and liaison for EDI efforts between PSD and PME

PME Faculty Ombudsperson — U. Chicago
Faculty Ombudsperson — 2020-present

- Departmental resource for confidential discussion and support regarding workplace problems

Faculty Diversity Liaisons — U. Chicago
Committee Member and PME Representative — 2020-present

- Provost's committee to advise and coordinate on campus-level EDI initiatives, priorities, and concerns

Vice Dean for Equity, Diversity, and Inclusion — U. Chicago
Member of PME Executive Council — 2020-present

- Faculty advocate, leader, and liaison for EDI efforts

Director of PME Master of Science Program — U. Chicago
Inaugural Faculty Program Director — 2020-2021

- Program director and architect of Computational Materials Modeling track

Faculty Search Committee — U. Chicago
Member — 2018-21

- Member of the PME faculty search committee

College Council Member — U. Chicago
PME Faculty Representative — 2019-20

- Exercise the legislative powers of the College Faculty in accordance with the Statutes of the University

Research Computing Center (RCC) Resource Allocation Committee — U. Chicago
Committee Member — 2019-present

- Review faculty proposals and allocate service units on RCC supercomputing resources

Research Computing Center (RCC) Faculty Education Advisory Committee — U. Chicago
PME Faculty Representative — 2019

- Review, revise, and develop the educational services and programs of the RCC

Center for Data and Computing (CDAC) Steering Committee — U. Chicago
Inaugural Steering Committee Member — 2018-20

- Provost's initiative to be an intellectual hub and incubator for interdisciplinary, computing and data-driven research

Reviews

Manuscript Reviews

- ACS Central Science (5), ACS Nano (2), ACS Synthetic Biology (1), AIMS Materials Science (1), Chem (1), Chem. Phys. (1), Chem. Phys. Lett. (1), Chemical Reviews (1), Chemical Science (2), Current Opinion in Chemical Engineering (1), eLife (1 as guest editor), Energy & Fuels (2), ICML2023 (2), Information Fusion (1), J. Chem. Eng. Data (1), J. Chem. Phys. (15), J. Chem. Theory Comput. (4), J. Comput. Phys. (1), J. Mol. Graph. Model. (5), J. Phys. Chem. (19), J. Phys. Chem. Letters (2), J. Phys. D (1), J. Polymer Science (1), J. Process Control (1), J. R. Soc. Interface (1), J. Supercrit. Fluids. (1), Langmuir (2), Macromolecules (2), Mol. Sim. (2), Mol. Sys. Des. Eng. (11), Molecular Modeling and Simulation (1), Nanoscale (1), Nature (1), Nature Communications (2), Nature Materials (1), npj Computational Materials (1), Physical Biology (1), Physical Review Research (1), PLOS Comput. Biol. (1), PLOS ONE (1), PNAS (8 + 3 as guest editor), PRL (3), PRX (2), Protein and Cell (1), RSC Advances (1), Science (3), Science Advances (1), Soft Matter (3), J. Cryst. Growth (1)

Proposal Reviews

Mail-in:

- NSF: DBI (1), DMR (19), CHE (4), ACI (2), CBET (1) *including* Postdoctoral Research Fellowship in Biology (PRFB) (1), RUI (1), CAREER (7), CDS&E (2), DIBB (2), LEAPS (1), CCI (1)
- DOE BES (5)
- Established Program to Stimulate Competitive Research (EPSCoR) (2)
- Biotechnology and Biological Sciences Research Council (BBSRC) (2)
- ACS PRF (8)
- National Academies workshop proceedings – Data Science: Opportunities to Transform Chemical Sciences and Engineering: Proceedings of a Workshop—in Brief
- 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)
- Army Research Office (1)
- DOE Office of Science Graduate Student Research (1)
- CECAM Workshop Proposal (1)

Panel:

- NSF (4)

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)
- Blue Waters Graduate Fellowship Program (5)
- University of Chicago Center for Data and Computing (CDAC) Data Science Discovery Grants (5)

External Thesis Committees

Bernadette Mohr, University of Amsterdam 2019-2023
Advisors: Peter Bolhuis, Tristan Bereau

Heather Aitken, Australian National University 2021
Advisor: Luke Connal

Online Educational Content

Generative AI in Science and Research

- Part of the UChicago Generative AI Video Series https://youtu.be/GtouQW75yUE?si=jhAD8fzqTQkOo-EB

Understanding Fracture Behavior in Materials Using Cheese
J.A. Krogstad, N.E. Johnson-Glauch, K. Tyler, R.A. Mansbach, and A.L. Ferguson (2018)

- Finite element method workshop designed for Girls Learning About Materials (GLAM) summer camp at UIUC https://nanohub.org/resources/28588

Elements of Integrated Computational Materials Engineering – Molecular Dynamics with LAMMPS

- Lectures and Course Materials: https://www.youtube.com/watch?v=N2L6jcMm3fI

MSE 498 – Computational Materials Science and Engineering

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

ACADEMIC HONORS AND AWARDS

Professorial ACMM Chair of Computational Science	U. Amsterdam	2022 – 2023
Dreyfus Foundation Machine Learning in the Chemical Sciences and Engineering Award	U. Chicago	2020
National Academy of Engineering / Alexander von Humboldt German-American Frontiers of Engineering Symposium Invitee	U. Chicago	2019
Journal of Process Control – Best Referee	U. Chicago	2018
IChemE Junior Moulton Medal	U. Chicago	2018/19
Royal Society of Chemistry Molecular Systems Design and Engineering Emerging Investigator Award	U. Chicago	2018
List of Teachers Ranked Outstanding by their Students	UIUC	2018 (Spring)
List of Teachers Ranked Outstanding by their Students	UIUC	2017 (Fall)
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 – 2024
Member of the American Institute of Chemical Engineers (AIChE)	2008 – present
Member of the American Chemical Society (ACS)	2012 – present

POSTDOCTORAL RESEARCH ADVISEES

Current

Dr. Siva Dasetty (PME, U. Chicago)	2020 – present
Dr. Armin Shayesteh Zadeh (PME, U. Chicago)	2023 – present
Dr. Soumajit Dutta (PME, U. Chicago)	2023 – present
Dr. Siddarth Achar (PME, U. Chicago)	2024 – present

Graduates

Dr. Hythem Sidky (PME, U. Chicago) 2018 – 2019
→ Senior Data Scientist, Kaiser Permanente
(Departed 07/15/19)

Dr. Brandon Peters (PME, U. Chicago) 2018 – 2019
→ Postdoctoral Appointee, Argonne National Lab
(Departed 12/09/19)

Dr. Mingfei Zhao (PME, U. Chicago) 2019 – 2022
→ Postdoctoral Fellow, Los Alamos National Lab
(Departed 08/31/22)

DOCTORAL RESEARCH ADVISEES

Current

Max Topel (PME, U. Chicago)	2020 – present
Yifeng (Oliver) Tang (PME, U. Chicago) – co-advised w/ Aaron Esser-Kahn	2020 – present
Nicholas Herringer (Chemistry, U. Chicago)	2020 – present
Kate Johnson (PME, U. Chicago) – co-advised w/ Nicolas Chevrier	2020 – present
Nikša Praljak (Biophysical Sciences, U. Chicago) – co-advised with Rama Ranganthan	2020 – present
Jianming Mao (Chemistry, U. Chicago)	2022 – present
Alex Berlaga (Chemistry, U. Chicago)	2022 – present
Hugh Yeh (MSTP, U. Chicago) – co-advised with Jun Huang	2023 – present
Marcia Luna Ramirez Hincapie (PME, U. Chicago)	2023 – present
Aniruddha Seal (Chemistry, U. Chicago)	2023 – present
Olabisi Bello (Chemistry, U. Chicago) – co-advised w/ Aaron Esser-Kahn	2024 – present
Sun Yong Kwon	2024 – present
Srivarshini Ganesan	2024 – present
Max Gruschka	2024 – present

Graduates

Andrew W. Long (MatSE, UIUC) 2012 – 2017
PhD Title: "Inverse design of self-assembling colloids via landscape engineering" (Defended 08/16/17)
→ Senior Data Scientist, Business and Safety Graphics Lab, 3M

Greg A. Hart (Physics, UIUC) 2012 – 2017
PhD Title: "*In silico* vaccine design for hepatitis C: A computational platform for fighting disease" (Defended 08/24/17)

→ Postdoctoral Associate w/ Prof. Jun Deng, Therapeutic Radiology, Yale School of Medicine
→ Research Scientist, Institute for Disease Modeling, Bill & Melinda Gates Foundation

Jiang Wang (Physics, UIUC) 2013 – 2018
PhD Title: "Nonlinear machine learning of macromolecular folding and self-assembly" (Defended 05/01/18)
→ Postdoctoral Associate w/ Profs. Cecilia Clementi and Frank Noé, Rice University
→ Teaching Staff (Assistant Professor equivalent), Department of Physics, Guizhou Institute of Technology (Commenced 12/01/20)

Rachael A. Mansbach (Physics, UIUC) 2014 – 2018
PhD Title: "Dimensionality reduction and multiscale modeling for the understanding of protein folding and hierarchical self-assembly" (Defended 05/08/18)
→ Director's Postdoctoral Fellow w/ Dr. Sandrasegaram Gnanakaran, Los Alamos National Lab
→ Assistant Professor of Physics, Concordia University (Commenced 08/01/20)

Bryce A. Thurston III (Physics, UIUC) 2013 – 2018
PhD Title: "Composition, thermodynamics, and morphology: A multi-scale computational approach for the design of self-assembling peptides" (Defended 10/23/18)
→ Postdoctoral Associate w/ Drs. Gary Grest, Amalie Frischknecht, and Mark Stevens, Sandia National Lab

Wei Chen (Physics, UIUC) 2015 – 2020
PhD Title: "Machine learning of molecular conformations, kinetics, and beyond" (Defended 10/23/18)
→ Data Scientist, Teza Technologies LLC

Yutao Ma (Physics, UIUC / PME, U. Chicago) 2017 – 2022
PhD Title: "Data-driven design of self-assembling soft materials" (Defended 05/27/22)
→ Risk Engineer, Goldman Sachs Inc.

Walter Alvarado (Biophysical Sciences, U. Chicago) – co-advised w/ Juan de Pablo 2019 – 2023
PhD Title: "Understanding the role and dynamics of nucleosomal organization" (Defended 07/10/23)
→ Junior Scientist, NASA

Kirill Shmilovich (PME, U. Chicago) 2019 – 2023
PhD Title: "Data-driven approaches for molecular design and simulation: From self-assembling peptides to enhanced sampling techniques and atomistic structure generation" (Defended 07/13/23)
→ Machine Learning Scientist, Genentech

Xinran Lian (Chemistry, U. Chicago) – co-advised w/ Rama Ranganathan 2019 – 2023
PhD Title: "Data-driven interpretation and design of orthologs and paralogs of a signaling protein" (Defended 12/01/23)
→ Postdoctoral Associate w/ Dr. Arvind Ramanathan, Argonne National Lab

Shiqi Chen (Chemistry, U. Chicago) – co-advised w/ Norbert Scherer 2019 – 2024
PhD Title: "Data-Driven Statistical Mechanical and Symmetry Insights into Collective Coordinates in Small Optical Matter Clusters" (Defended 05/31/24)
→ Postdoctoral Associate w/ Prof. Jason R. Green, UMass Boston

Mike Jones (PME, U. Chicago) 2020 – 2024
PhD Title: "Deep Learning Approaches to Extend Time and Length Scales of Molecular Simulations" (Defended 10/24/24)
→ Postdoctoral Associate w/ Drs. Kelli Humbird and Felice Lightstone, Design Physics Division, Lawrence Livermore National Laboratory

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

MASTER'S RESEARCH ADVISEES

Sascha Frey (Robotics, EPFL) Spring 2020

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 – 2018
Chin-Yu "Chester" Cheng (ECE, UIUC)	2016 – 2018
Aik Rui Tan (MatSE, UIUC)	2017 – 2018
Aditi Munshi (CS, Grinnell College)	Summer 2017
Marlo Zorman (Chem, University of Vermont)	Summer 2018
Isabelle Augensen (CS, CMU)	Summer 2018
Olivia Dunne (PME, U. Chicago)	2018 – 2020
Gillian Shen (Chem, U. Chicago)	2018 – 2020
Joseph Aulicino (PME, U. Chicago)	2019 – 2021
Jaycie Mundell (Rock Valley College)	Summer 2019
Xiyi Chen (CS, U. Maryland)	Summer 2019
Yuanbo Zhang (CS, UW Madison)	Summer 2019
Melody Leung (PME, U. Chicago)	2020 – 2022
Antony Awad (PME, U. Chicago)	Summer 2020
Rohan Kapoor (PME, U. Chicago)	2021 – 2022
Sebastian Suarez Schmidt (Physics, University of Puerto Rico-Rio Piedras)	Summer 2021
Milla Venasen (ChemE, University of Texas at San Antonio)	Summer 2021
Brenna Bartholomew (ChemE, University of Virginia)	Summer 2021
Smayan Khanna (PME, U. Chicago)	2022 – 2024
Junhee Lee (PME, U. Chicago)	2022 – present
Diya Ganhdi (PME, U. Chicago)	2022 – 2024
Aidan Rambo (Xavier University of Louisiana)	Summer 2023
Jay Shen (Physics and Computer Science, U. Chicago)	2023 – present
Abhiraman Senthilkumar (CS, U. Maryland)	Summer 2024
Srusti Donapati (Biological Science and Data Science, UChicago)	2024 – present
Tommy Walsh (Biology and Computer Science, UChicago)	2024 – present

HIGH SCHOOL RESEARCH ADVISEES

Yvette Hernandez (PME After School Matters STEM Lab Internship Program)	Summer 2019
Isabella Moughal (PME After School Matters STEM Lab Internship Program)	Summer 2019
Camilla Forero (PME After School Matters STEM Lab Internship Program)	2024 – present

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
8. 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
9. NSF/DMR/CMMT, NSF/DMS/Statistics, "MATDAT18: Materials and Data Sciences Hackathon" (Grant No. DMR-1748198), PI: B. Reich (NCSU), Co-PIs: T. Mueller (JHU), S. Rajasekaran (UConn), A.L. Ferguson (UofC), Total Award: $148,810 ($9,107 to Ferguson), 08/01/17 – 07/31/18
10. DOE (Argonne National Laboratory Subcontract), "MICCoM: Midwest Center for Computational Materials" (Argonne National Laboratory, DOE Prime Contract No. DE-AC02-06CH11357), PI: G. Galli (UofC), J.J. de Pablo (UofC), M. Govoni (UofC, Argonne), F. Gygi (UC Davis), J. Whitmer (Notre Dame), Total Award: $1,149,859 ($80,000 to Ferguson), 07/31/18 – 07/31/19
11. Zoetis, "Atomic level molecular simulations by GROMACS software package", PIs: A.L. Ferguson (UofC), N. Deng (Zoetis), Total Award: $34,767 ($34,767 to Ferguson), 11/01/18 – 12/31/19
12. 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 (UofC), J. Peng (UIUC), J. Byrd (UIUC), M. Snir (UIUC), Total Award: $360,036, 03/01/17 – 02/28/20
13. NSF/DMR/CMMT, "CAREER: Teaching Machines to Design Self-Assembling Materials" (Grant No. DMR-1841800), PI: A.L. Ferguson (UofC), Total Award: $450,000 ($450,000 to Ferguson), 06/01/14 – 05/31/20
14. University of Chicago Center for Data and Computing (CDAC) Data Science Discovery Grants Winter 2019, "Rational protein engineering using data-driven generative models", PI: A.L. Ferguson (UofC), Co-PI: R. Ranganathan (UofC), Total Award: $85,102, 04/15/19 – 05/31/20
15. University of Chicago Innovation District Collaborative Research Initiative (IDCRI) Seed Funding, "Computationally Evolved 2D Peptide Assemblies", PIs: C. Fry (ANL), S. Sankaranaryanan (ANL), A.L. Ferguson (UofC), Total Award: $35,000, 10/16/19 – 04/15/20
16. NSF/MPS/DMS/Mathematical Biology, "Nonlinear Manifold Learning of Protein Folding Funnels From Delay-Embedded Experimental Measurements" (Grant No. DMS-1841810), PI: A.L. Ferguson (UofC), Total Award: $210,000 ($210,000 to Ferguson), 08/01/17 – 07/31/21
17. NSF/DMR/CMMT, "EAGER: Collaborative Research: Type II: Data-Driven Characterization and Engineering of Protein Hydrophobicity" (Grant No. DMR-1844505), PIs: A.L. Ferguson (UofC), A. Patel (UPenn), Total Award: $284,629 ($52,982 to Ferguson), 09/01/18 – 12/31/21
18. Indo-U.S. Science and Technology Forum, "Recent Advances in Machine-Learning Tools for Studying Rare Events in Molecular Simulations" (Ref: IUSSTF/AUG/WS/140/2019), PIs: A. Chandra (IIT Kanpur), A.L. Ferguson (UofC); Co-PIs: J. Mondal (Tata Institute of Fundamental Research), P. Tiwary (University of Maryland), Total Award: $18,000, 12/09/20 – 12/12/21
19. NSF/CHE/CTMC, "Nonlinear Dimensionality Reduction and Enhanced Sampling in Molecular Simulation Using Auto-Associative Neural Networks" (Grant No. CHE-1841805), PI: A.L. Ferguson (UofC), Total Award: $380,105 ($380,105 to Ferguson), 06/15/17 – 05/31/22
20. DOD/ARO (W911NF-17-S-0002-06), "Workshop on Data-Driven Design of Heterogeneous Materials" (Grant No. W911NF-17-S-0002-06), PI: A.L. Ferguson (UofC); Co-PI: J.J. de Pablo (UofC), Total Award $21,532, 07/01/2020 – 06/30/2022
21. NSF/DMR/BMAT, "EAGER: Collaborative Research: Exploring the emergence of peptide-based compartments through iterative machine learning, molecular modeling, and cell-free protein synthesis" (Grant No. DMR-

1939463), PI: A. Ferguson (UofC), A. Liu (U. Michigan), Total Award $299,902 ($149,902 to Ferguson), 08/15/2019 – 07/31/2022

22. DOE/BES/EFRC, "CSSAS: The Center for the Science of Synthesis Across Scales" (Grant No. DE-SC0019288), PI: F. Baneyx (UW), Senior Personnel: M. Baer (PNNL), D. Baker (UW), D. Beck (UW), C.-L. Chen (PNNL), B. Cossairt (UW), J. De Yoreo (PNNL), A.L. Ferguson (U. Chicago), D. Ginger (UW), S. Jenekhe (UW), S. Kalinin (ORNL), C. Mundy (PNNL), J. Pfaendtner (UW), A. Tezcan (UCSD), Total Award: $10,750,000 ($430,001 to Ferguson), 08/01/18 – 07/31/22
23. Chan Zuckerberg Initiative, "Decoding Inter-Organ Inflammatory Signaling at the Single-Cell Level", PI: N. Chevrier (UofC); Co-PI: S. Tay (UofC), A.L. Ferguson (UofC), Total Award $525,000 ($175,000 to Ferguson), 09/01/2020 – 08/31/2022
24. DOE (Argonne National Laboratory Subcontract), "MICCoM-2 Center (Argonne Work Order 21D)" (Grant No. 5J-30161-0021A, Renewal #1), PI: G. Galli (UofC), Co-I: J.J. de Pablo (UofC), M. Govoni (UofC, Argonne), F. Gygi (UC Davis), J. Whitmer (Notre Dame), A.L. Ferguson (UofC), M. Chan (Argonne), J. Heremans (UofC, Argonne), D. Talapin (UofC), Total Award: $10,000,000 ($240,000 to Ferguson), 08/01/19 – 07/31/23
25. NSF/DMR/DMREF, "DMREF: Collaborative Research: Self-Assembled Peptide-Pi-Electron Supramolecular Polymers for Bioinspired Energy Harvesting, Transport and Management" (Grant No. DMR-1841807), PI: J.D. Tovar (JHU), Co-PIs: H.E. Katz, (JHU), A.L. Ferguson (UofC), Total Award: $1,600,000 ($536,783 to Ferguson), 07/01/17 – 09/30/23
26. NIH/NIAID Vaccine Adjuvant Discovery Program, "Discovery of Adjuvants via Novel Modulation of Innate Immune Pathways for Vaccines Against Influenza" (Contract Number: 75N93019C00041, NIAID Reference Number: NIAID-DAIT-NIHAI201700100), PI: A. Esser-Kahn (UofC), Co-PIs: J. Hubbell (UofC), A. Chong (UofC), M. Kwissa (UofC), S. Tay (UofC), A.L. Ferguson (UofC), S. Chen (UofC), P. Felgner (UC Irvine), H. Davies (UC Irvine), A. Burkhardt (UC Irvine), R. Baker (IITRI), D. Boltz (IITRI), Total Award: $7,506,602, 09/30/19 – 09/30/24
27. Camille and Henry Dreyfus Foundation Program for Machine Learning in the Chemical Sciences and Engineering, "Data-driven protein engineering using deep generative learning and high-throughput gene synthesis (Grant No. ML-20-157)", PI: A.L. Ferguson (UofC); Co-PI: R. Ranganathan (UofC), Total Award $140,000, 09/01/2020 – 08/31/2024

Current Support

1. NSF/CHE/CTMC, "Latent space simulators for the efficient estimation of long-time molecular thermodynamics and kinetics" (Grant No. CHE-2152521), PI: A.L. Ferguson (UofC), Total Award: $387,874, 04/01/22 – 03/31/25
2. NSF/MRSEC-PREM "Xavier-UChicago Partnership for Research and Education in Materials for Energy Storage and Sensing" (Grant No. DMR-2122058), PI: A. Abdulahad (Xavier University of Louisiana), M. Gardel (UofC), Total Award: $750,000, 09/01/21 – 08/30/27
3. NSF/EEC/EWFD, "REU SITE: Research Experience for Undergraduates in Molecular Engineering" (Grant No. EEC-2050878), PI: A.L. Ferguson; Co-PI: J.J. de Pablo (UofC); Senior Personnel: C. Amanchukwu (UofC), G. Galli (UofC), M. Gardel (UofC), A. High (UofC), C. Liu (UofC), J. Mendoza (UofC), S. Rowan (UofC), A. Squires (UofC), M. Swartz (UofC), T. Zhong (UofC), Total Award $434,002, 04/15/2021 – 03/14/2025
4. NSF/NRT – NSF Research Traineeship Program, "NRT-HDR: AI-enabled Molecular Engineering of Materials and Systems (AIMEMS) for Sustainability and Medical Applications" (Grant No. DGE-2022023), PI: J.J. de Pablo (UofC); Co-PI: R. Willett (UofC), M. Gardel (UofC), P. Nealey (UofC), J. Cheng (UofC); Senior Personnel: R. Stevens (UofC), A.L. Ferguson (UofC), S. Patel (UofC), J. Evans (UofC), Total Award $3,000,000, 09/01/2020 – 08/31/2025
5. DOE/BES/EFRC, "CSSAS: The Center for the Science of Synthesis Across Scales (Grant No. DE-SC0019288)", PI: F. Baneyx (UW), Senior Personnel: J. De Yoreo (PNNL), A.L. Ferguson (U. Chicago), B. Cossairt (UW), L. Pozzo (UW), D. Baker (UW), C.-L. Chen (PNNL), O. Gang (Columbia), D. Ginger (UW), S. Jenekhe (UW), S. Kalinin (UT Knoxville), C. Mundy (PNNL), J. Pfaendtner (UW), W. Shaw (PNNL), A. Tezcan (UCSD), S. Zhang (UW), Total Award: $16,000,000 ($680,000 to Ferguson), 08/01/22 – 07/31/26
6. DOE/BES/EFRC, "Catalyst Design for Decarbonization Center (CD4DC) (Grant No. DE-SC0023383)", PI: L. Gagliardi (UChicago), Senior Personnel: C. Amanchukwu (UChicago), J. Anderson (UChicago), K. Chapman (Stony Brook University), M. Delferro (ANL), J.J. de Pablo (UChicago), O. Farha (Northwestern), A.L. Ferguson (UChicago), I. Foster (UChicago), R. Getman (Clemson), K. Glusac (UIC), J. Hupp (Northwestern), M. Neurock (U. Minnesota), J. Notestein (Northwestern), J. Lercher (PNNL), D. Truhlar (U. Minnesota), N. Washton (PNNL), A. Wuttig (UChicago), Total Award: $12,450,000, 08/01/22 – 07/31/26
7. DOE/BES/CCS, "Multiscale Computational Framework for Biomolecular Energy Transduction: From Electrons to the Mesoscale (Grant No. DE-SC0023318)", PIs: G.A. Voth (UofC), Co-PIs: A.L. Ferguson (UofC), G. Chan

(CalTech), T. Bidone (Utah), C.J. Knight (Argonne), S. Plimpton (Sandia), Total Award: $2,897,643 ($428,517 to Ferguson), 09/01/22 – 08/31/25

8. UChicago MRSEC Proto-IRG, "Leveraging Organic Ionic Plastic Crystals (OIPCs) Towards Unconventional Crystalline Soft Materials (Grant No. DMR-2011854)", PI: S. Patel (UofC), Co-PIs: C. Amanchukwu (UofC), S.J. Rowan (UofC), J.J. de Pablo (UofC), A.L. Ferguson (UofC), Total Award: $80,000, 09/01/20 – 08/31/26
9. ARO/Life Sciences/Biochemistry/Bimolecular Assembly and Organization, "Design of self-organizing peptide chassis materials for synthetic cells by machine learning, molecular modeling, and cell-free protein synthesis (Grant No. W911NF-23-1-0050)", PI: A.L. Ferguson (UofC) (collaboration w/ Allen Liu (U. Michigan)), Total Award: $314,712, 04/01/23 – 03/31/26
10. ARO/Materials Design, "High-throughput virtual screening and hybrid computational/experimental active learning for novel hydrogel-nanoparticle sensors (Grant No. W911NF-23-2-0135), PI: A.L. Ferguson (UofC), Total Award: $278,186, 06/01/23 – 05/31/25
11. DOE (Argonne National Laboratory Subcontract), "MICCoM-3 Center (Grant No. 3F-60244)", PI: G. Galli (UofC), Co-I: J.J. de Pablo (UofC), M. Govoni (UofC, Argonne), F. Gygi (UC Davis), J. Whitmer (Notre Dame), A.L. Ferguson (UofC), M. Chan (Argonne), J. Heremans (UofC, Argonne), J. Xu (Argonne), Total Award: $9,000,000, 09/01/23 – 08/31/26
12. NSF/DMR/DMREF, "Collaborative Research: DMREF: Closed-Loop Design of Polymers with Adaptive Networks for Extreme Mechanics (Grant No. DMR-2323727)", PI: C, Ke (Dartmouth), Co-PIs: K. Brown (BU), R. Smaldone (UT Dallas), G. Gu (Berkeley), A.L. Ferguson (UofC), Total Award: $1,998,559 ($421,781 to Ferguson), 10/01/23 – 09/31/27
13. NIAID, "Discovery of Adjuvants that Direct T-cell Fates for Improved Safety and Efficacy in Vaccines Against Influenza (Proposal No. FP110241)", PI: A. Esser-Kahn (UofC), Co-PIs: J. Hubbell (UofC), J. Huang (UofC), M. Swartz (UofC), S. Khader (UofC), A.L. Ferguson (UofC), E. Xu (UofC), J. Tomalka (Emory), Total Award: $9,807,060 , 09/01/24 – 09/30/29

Pending Support

1. Office of Naval Research/DURIP, "High Performance Computer for Materials Modeling and Design (Proposal No. FP110669)", PI: L. Gagliardi (UofC), G. Voth (UofC), G. Galli (UofC), A.L. Ferguson (UofC), J. de Pablo (UofC), D. Mazziotti (UofC), Total Award: $1,249,999, 12/01/24 – 11/30/29
2. NSF/DMR/CMMT, "Collaborative Research: Learning How Nanoscale Chemical and Topographical Patterning Influences Hydrophobicity", PIs: A.P. Patel (UPenn), A.L. Ferguson (UofC), Total Award: $712,661 ($117,168 to Ferguson), 09/01/24 – 08/31/28
3. NSF/EEC/EWFD, "REU SITE: Research Experience for Undergraduates in Molecular Engineering" (Proposal No. FP114407), PI: A.L. Ferguson; Co-PI: N. Mason (UofC), Total Award $515,408, 04/01/2025 – 03/31/2028
4. NSF, "ReNew: AI/ML-assisted Design of Field-effect Transistor (FET) Sensors for Detecting Per- and Polyfluoroalkyl Substances (PFAS) and Cobalt (II) Ions in Water" (Proposal No. FP113463), PI: J. Chen (UofC), Co-PIs: A.L. Ferguson (UofC), S. Darling (Argonne), Total Award: $647,074, 07/01/24 – 06/30/26
5. NSF, "NSF Engine: The Synthetic Biology and Artificial Intelligence Midwest Anti-infectives Design and Engineering (SynBio MADE)", PI: H. Hoffman (UofC), Total Award: $600,000, 03/01/26 – 02/28/36
6. NSF, "Collaborative Research: DMREF: Unlocking the effect of Angstrom-scale confinement on oligopeptide binding to metal ions for critical element separation", PI: C. Liu (UofC), Co-PI: G. Schatz (Northwestern), Senior Personnel: M. Tirrell (UofC), A.L. Ferguson (UofC), Total Award: $1,400,000, 09/01/25 – 08/31/29