Andrew Ferguson

List of Publications by Year in Descending Order

86 papers	3,228 citations	33 h-index	55 g-index
101 ext. papers	4,191 ext. citations	6.2 avg, IF	6.03 L-index

#	Paper	IF	Citations
86	Data-Driven Design and Autonomous Experimentation in Soft and Biological Materials Engineering.. *Annual Review of Chemical and Biomolecular Engineering*, **2022**,	8.9	1
85	Facile formation of giant elastin-like polypeptide vesicles as synthetic cells. *Chemical Communications*, **2021**, 57, 13202-13205	5.8	1
84	Determining Sequence-Dependent DNA Oligonucleotide Hybridization and Dehybridization Mechanisms Using Coarse-Grained Molecular Simulation, Markov State Models, and Infrared Spectroscopy. *Journal of the American Chemical Society*, **2021**, 143, 17395-17411	16.4	5
83	PACAP is a pathogen-inducible resident antimicrobial neuropeptide affording rapid and contextual molecular host defense of the brain. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	9
82	Inverse Design of Self-Assembling Diamond Photonic Lattices from Anisotropic Colloidal Clusters. *Journal of Physical Chemistry B*, **2021**, 125, 2398-2410	3.4	3
81	Near quantitative synthesis of urea macrocycles enabled by bulky N-substituent. *Nature Communications*, **2021**, 12, 1572	17.4	4
80	Data-driven reaction coordinate discovery in overdamped and non-conservative systems: application to optical matter structural isomerization. *Nature Communications*, **2021**, 12, 2548	17.4	2
79	Tetranucleosome Interactions Drive Chromatin Folding. *ACS Central Science*, **2021**, 7, 1019-1027	16.8	5
78	Computationally Guided Tuning of Peptide-Conjugated Perylene Diimide Self-Assembly. *Langmuir*, **2021**, 37, 8594-8606	4	3
77	Pushing and Pulling: A Dual pH Trigger Controlled by Varying the Alkyl Tail Length in Heme Coordinating Peptide Amphiphiles. *Journal of Physical Chemistry B*, **2021**, 125, 1317-1330	3.4	2
76	Accelerated polymerization of N-carboxyanhydrides catalyzed by crown ether. *Nature Communications*, **2021**, 12, 732	17.4	11
75	100th Anniversary of Macromolecular Science Viewpoint: Data-Driven Protein Design.. *ACS Macro Letters*, **2021**, 10, 327-340	6.6	5
74	// Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry B*, **2020**, 124, 9767-9772	3.4	2
73	// Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry A*, **2020**, 124, 9113-9118	2.8	1
72	The Journal of Physical Chemistry A/B/C Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry C*, **2020**, 124, 24033-24038	3.8	1
71	Statistically Optimal Continuous Free Energy Surfaces from Biased Simulations and Multistate Reweighting. *Journal of Chemical Theory and Computation*, **2020**, 16, 4107-4125	6.4	3
70	Computationally Guided Tuning of Amino Acid Configuration Influences the Chiroptical Properties of Supramolecular Peptide-Peptide Nanostructures. *Langmuir*, **2020**, 36, 6782-6792	4	4

69	Machine Learning Force Fields and Coarse-Grained Variables in Molecular Dynamics: Application to Materials and Biological Systems. *Journal of Chemical Theory and Computation*, **2020**, 16, 4757-4775	6.4	46
68	Discovery of Self-Assembling -Conjugated Peptides by Active Learning-Directed Coarse-Grained Molecular Simulation. *Journal of Physical Chemistry B*, **2020**, 124, 3873-3891	3.4	37
67	Machine learning for collective variable discovery and enhanced sampling in biomolecular simulation. *Molecular Physics*, **2020**, 118, e1737742	1.7	41
66	The value of antimicrobial peptides in the age of resistance. *Lancet Infectious Diseases, The*, **2020**, 20, e216-e230	25.5	243
65	Effect of Core Oligomer Length on the Phase Behavior and Assembly of -Conjugated Peptides. *ACS Applied Materials & Interfaces*, **2020**, 12, 20722-20732	9.5	2
64	Reconstruction of protein structures from single-molecule time series. *Journal of Chemical Physics*, **2020**, 153, 194102	3.9	1
63	Free energy calculations of the functional selectivity of 5-HT2B G protein-coupled receptor. *PLoS ONE*, **2020**, 15, e0243313	3.7	2
62	In search of a novel chassis material for synthetic cells: emergence of synthetic peptide compartment. *Soft Matter*, **2020**, 16, 10769-10780	3.6	2
61	MARTINI-Compatible Coarse-Grained Model for the Mesoscale Simulation of Peptoids. *Journal of Physical Chemistry B*, **2020**, 124, 7745-7764	3.4	10
60	Molecular latent space simulators. *Chemical Science*, **2020**, 11, 9459-9467	9.4	12
59	High-Resolution Markov State Models for the Dynamics of Trp-Cage Miniprotein Constructed Over Slow Folding Modes Identified by State-Free Reversible VAMPnets. *Journal of Physical Chemistry B*, **2019**, 123, 7999-8009	3.4	20
58	Capabilities and limitations of time-lagged autoencoders for slow mode discovery in dynamical systems. *Journal of Chemical Physics*, **2019**, 151, 064123	3.9	13
57	Polymeric "Clickase" Accelerates the Copper Click Reaction of Small Molecules, Proteins, and Cells. *Journal of the American Chemical Society*, **2019**, 141, 9693-9700	16.4	50
56	Synthesis of polypeptides via bioinspired polymerization of in situ purified -carboxyanhydrides. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 10658-10663	11.5	52
55	Nonlinear discovery of slow molecular modes using state-free reversible VAMPnets. *Journal of Chemical Physics*, **2019**, 150, 214114	3.9	38
54	Controlling Supramolecular Chirality in Peptide-Peptide Networks by Variation of the Alkyl Spacer Length. *Langmuir*, **2019**, 35, 14060-14073	4	15
53	Revealing the Sequence-Structure-Electronic Property Relation of Self-Assembling -Conjugated Oligopeptides by Molecular and Quantum Mechanical Modeling. *Langmuir*, **2019**, 35, 15221-15231	4	5
52	Inverse design of self-assembling colloidal crystals with omnidirectional photonic bandgaps. *Soft Matter*, **2019**, 15, 8808-8826	3.6	14

51	Landmark diffusion maps (L-dMaps): Accelerated manifold learning out-of-sample extension. *Applied and Computational Harmonic Analysis*, **2019**, 47, 190-211	3.1	17
50	A Study of the Morphology, Dynamics, and Folding Pathways of Ring Polymers with Supramolecular Topological Constraints Using Molecular Simulation and Nonlinear Manifold Learning. *Macromolecules*, **2018**, 51, 598-616	5.5	10
49	Machine learning-enabled discovery and design of membrane-active peptides. *Bioorganic and Medicinal Chemistry*, **2018**, 26, 2708-2718	3.4	45
48	Rational design of patchy colloids via landscape engineering. *Molecular Systems Design and Engineering*, **2018**, 3, 49-65	4.6	23
47	Machine learning and molecular design of self-assembling -conjugated oligopeptides. *Molecular Simulation*, **2018**, 44, 930-945	2	18
46	Computational design of hepatitis C virus immunogens from host-pathogen dynamics over empirical viral fitness landscapes. *Physical Biology*, **2018**, 16, 016004	3	12
45	Nonlinear machine learning in simulations of soft and biological materials. *Molecular Simulation*, **2018**, 44, 1090-1107	2	17
44	Machine learning and data science in soft materials engineering. *Journal of Physics Condensed Matter*, **2018**, 30, 043002	1.8	73
43	Recovery of Protein Folding Funnels from Single-Molecule Time Series by Delay Embeddings and Manifold Learning. *Journal of Physical Chemistry B*, **2018**, 122, 11931-11952	3.4	6
42	Machine learning antimicrobial peptide sequences: Some surprising variations on the theme of amphiphilic assembly. *Current Opinion in Colloid and Interface Science*, **2018**, 38, 204-213	7.6	14
41	Molecular enhanced sampling with autoencoders: On-the-fly collective variable discovery and accelerated free energy landscape exploration. *Journal of Computational Chemistry*, **2018**, 39, 2079-2102	3.5	83
40	Patchy Particle Model of the Hierarchical Self-Assembly of -Conjugated Optoelectronic Peptides. *Journal of Physical Chemistry B*, **2018**, 122, 10219-10236	3.4	11
39	Enzyme-like Click Catalysis by a Copper-Containing Single-Chain Nanoparticle. *Journal of the American Chemical Society*, **2018**, 140, 13695-13702	16.4	57
38	Evidence for Prenucleated Fibrilogenesis of Acid-Mediated Self-Assembling Oligopeptides via Molecular Simulation and Fluorescence Correlation Spectroscopy. *Langmuir*, **2018**, 34, 7346-7354	4	7
37	Collective variable discovery and enhanced sampling using autoencoders: Innovations in network architecture and error function design. *Journal of Chemical Physics*, **2018**, 149, 072312	3.9	56
36	Coarse-Grained Molecular Simulation and Nonlinear Manifold Learning of Archipelago Asphaltene Aggregation and Folding. *Journal of Physical Chemistry B*, **2018**, 122, 6627-6647	3.4	11
35	Coarse-Grained Molecular Simulation of the Hierarchical Self-Assembly of -Conjugated Optoelectronic Peptides. *Journal of Physical Chemistry B*, **2017**, 121, 1684-1706	3.4	26
34	Mesoscale Simulation and Machine Learning of Asphaltene Aggregation Phase Behavior and Molecular Assembly Landscapes. *Journal of Physical Chemistry B*, **2017**, 121, 4923-4944	3.4	25

33	BayesWHAM: A Bayesian approach for free energy estimation, reweighting, and uncertainty quantification in the weighted histogram analysis method. *Journal of Computational Chemistry*, **2017**, 38, 1583-1605	3.5	35
32	Machine learning for autonomous crystal structure identification. *Soft Matter*, **2017**, 13, 4733-4745	3.6	64
31	Control of the hierarchical assembly of π-conjugated optoelectronic peptides by pH and flow. *Organic and Biomolecular Chemistry*, **2017**, 15, 5484-5502	3.9	14
30	What can machine learning do for antimicrobial peptides, and what can antimicrobial peptides do for machine learning?. *Interface Focus*, **2017**, 7, 20160153	3.9	54
29	Modulation of polypeptide conformation through donor-acceptor transformation of side-chain hydrogen bonding ligands. *Nature Communications*, **2017**, 8, 92	17.4	33
28	Molecular Motor Dnm1 Synergistically Induces Membrane Curvature To Facilitate Mitochondrial Fission. *ACS Central Science*, **2017**, 3, 1156-1167	16.8	17
27	Mesoscale Simulation of Asphaltene Aggregation. *Journal of Physical Chemistry B*, **2016**, 120, 8016-35	3.4	48
26	Nonlinear reconstruction of single-molecule free-energy surfaces from univariate time series. *Physical Review E*, **2016**, 93, 032412	2.4	19
25	Mapping membrane activity in undiscovered peptide sequence space using machine learning. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 13588-13593	11.5	87
24	Thermodynamics, morphology, and kinetics of early-stage self-assembly of π-conjugated oligopeptides. *Molecular Simulation*, **2016**, 42, 955-975	2	24
23	Global graph matching using diffusion maps. *Intelligent Data Analysis*, **2016**, 20, 637-654	1.1	6
22	Thermal Unthreading of the Lasso Peptides Astexin-2 and Astexin-3. *ACS Chemical Biology*, **2016**, 11, 3043-3051	4.9	33
21	Nonlinear machine learning and design of reconfigurable digital colloids. *Soft Matter*, **2016**, 12, 7119-35	3.6	18
20	Error catastrophe and phase transition in the empirical fitness landscape of HIV. *Physical Review E*, **2015**, 91, 032705	2.4	9
19	Helical antimicrobial polypeptides with radial amphiphilicity. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 13155-60	11.5	120
18	Machine learning assembly landscapes from particle tracking data. *Soft Matter*, **2015**, 11, 8141-53	3.6	44
17	Machine learning of single molecule free energy surfaces and the impact of chemistry and environment upon structure and dynamics. *Journal of Chemical Physics*, **2015**, 142, 105101	3.9	26
16	Empirical fitness models for hepatitis C virus immunogen design. *Physical Biology*, **2015**, 12, 066006	3	11

15	Supramolecular polymorphism: tunable electronic interactions within π-conjugated peptide nanostructures dictated by primary amino acid sequence. *Langmuir*, **2014**, 30, 5946-56	4	56
14	Nonlinear machine learning of patchy colloid self-assembly pathways and mechanisms. *Journal of Physical Chemistry B*, **2014**, 118, 4228-44	3.4	56
13	Investigating the optimal size of anticancer nanomedicine. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 15344-9	11.5	406
12	Variation of formal hydrogen-bonding networks within electronically delocalized π-conjugated oligopeptide nanostructures. *Langmuir*, **2014**, 30, 11375-85	4	26
11	The fitness landscape of HIV-1 gag: advanced modeling approaches and validation of model predictions by in vitro testing. *PLoS Computational Biology*, **2014**, 10, e1003776	5	93
10	Translating HIV sequences into quantitative fitness landscapes predicts viral vulnerabilities for rational immunogen design. *Immunity*, **2013**, 38, 606-17	32.3	160
9	Spin models inferred from patient-derived viral sequence data faithfully describe HIV fitness landscapes. *Physical Review E*, **2013**, 88, 062705	2.4	59
8	Computational prediction of broadly neutralizing HIV-1 antibody epitopes from neutralization activity data. *PLoS ONE*, **2013**, 8, e80562	3.7	15
7	A computational investigation of the phase behavior and capillary sublimation of water confined between nanoscale hydrophobic plates. *Journal of Chemical Physics*, **2012**, 137, 144501	3.9	36
6	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. *Chemical Physics Letters*, **2011**, 509, 1-11	2.5	103
5	Integrating diffusion maps with umbrella sampling: application to alanine dipeptide. *Journal of Chemical Physics*, **2011**, 134, 135103	3.9	55
4	Systematic determination of order parameters for chain dynamics using diffusion maps. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 13597-602	11.5	115
3	An experimental and computational investigation of spontaneous lasso formation in microcin J25. *Biophysical Journal*, **2010**, 99, 3056-65	2.9	51
2	Solubility and molecular conformations of n-alkane chains in water. *Journal of Physical Chemistry B*, **2009**, 113, 6405-14	3.4	116
1	Oxidation of hydroquinone to p-benzoquinone catalyzed by Cu(II) supported on chitosan flakes. *Journal of Applied Polymer Science*, **2006**, 100, 3034-3043	2.9	22