Andrew Ferguson

List of Publications by Citations

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	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
85	The value of antimicrobial peptides in the age of resistance. *Lancet Infectious Diseases, The*, **2020**, 20, e216-e230	25.5	243
84	Translating HIV sequences into quantitative fitness landscapes predicts viral vulnerabilities for rational immunogen design. *Immunity*, **2013**, 38, 606-17	32.3	160
83	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
82	Solubility and molecular conformations of n-alkane chains in water. *Journal of Physical Chemistry B*, **2009**, 113, 6405-14	3.4	116
81	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
80	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. *Chemical Physics Letters*, **2011**, 509, 1-11	2.5	103
79	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
78	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
77	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
76	Machine learning and data science in soft materials engineering. *Journal of Physics Condensed Matter*, **2018**, 30, 043002	1.8	73
75	Machine learning for autonomous crystal structure identification. *Soft Matter*, **2017**, 13, 4733-4745	3.6	64
74	Spin models inferred from patient-derived viral sequence data faithfully describe HIV fitness landscapes. *Physical Review E*, **2013**, 88, 062705	2.4	59
73	Enzyme-like Click Catalysis by a Copper-Containing Single-Chain Nanoparticle. *Journal of the American Chemical Society*, **2018**, 140, 13695-13702	16.4	57
72	Supramolecular polymorphism: tunable electronic interactions within π-conjugated peptide nanostructures dictated by primary amino acid sequence. *Langmuir*, **2014**, 30, 5946-56	4	56
71	Nonlinear machine learning of patchy colloid self-assembly pathways and mechanisms. *Journal of Physical Chemistry B*, **2014**, 118, 4228-44	3.4	56
70	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

69	Integrating diffusion maps with umbrella sampling: application to alanine dipeptide. *Journal of Chemical Physics*, **2011**, 134, 135103	3.9	55
68	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
67	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
66	An experimental and computational investigation of spontaneous lasso formation in microcin J25. *Biophysical Journal*, **2010**, 99, 3056-65	2.9	51
65	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
64	Mesoscale Simulation of Asphaltene Aggregation. *Journal of Physical Chemistry B*, **2016**, 120, 8016-35	3.4	48
63	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
62	Machine learning-enabled discovery and design of membrane-active peptides. *Bioorganic and Medicinal Chemistry*, **2018**, 26, 2708-2718	3.4	45
61	Machine learning assembly landscapes from particle tracking data. *Soft Matter*, **2015**, 11, 8141-53	3.6	44
60	Machine learning for collective variable discovery and enhanced sampling in biomolecular simulation. *Molecular Physics*, **2020**, 118, e1737742	1.7	41
59	Nonlinear discovery of slow molecular modes using state-free reversible VAMPnets. *Journal of Chemical Physics*, **2019**, 150, 214114	3.9	38
58	Discovery of Self-Assembling π-Conjugated Peptides by Active Learning-Directed Coarse-Grained Molecular Simulation. *Journal of Physical Chemistry B*, **2020**, 124, 3873-3891	3.4	37
57	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
56	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
55	Modulation of polypeptide conformation through donor-acceptor transformation of side-chain hydrogen bonding ligands. *Nature Communications*, **2017**, 8, 92	17.4	33
54	Thermal Unthreading of the Lasso Peptides Astexin-2 and Astexin-3. *ACS Chemical Biology*, **2016**, 11, 3043-3051	4.9	33
53	Coarse-Grained Molecular Simulation of the Hierarchical Self-Assembly of π-Conjugated Optoelectronic Peptides. *Journal of Physical Chemistry B*, **2017**, 121, 1684-1706	3.4	26
52	Variation of formal hydrogen-bonding networks within electronically delocalized π-conjugated oligopeptide nanostructures. *Langmuir*, **2014**, 30, 11375-85	4	26

51	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
50	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
49	Thermodynamics, morphology, and kinetics of early-stage self-assembly of -conjugated oligopeptides. *Molecular Simulation*, **2016**, 42, 955-975	2	24
48	Rational design of patchy colloids via landscape engineering. *Molecular Systems Design and Engineering*, **2018**, 3, 49-65	4.6	23
47	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
46	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
45	Nonlinear reconstruction of single-molecule free-energy surfaces from univariate time series. *Physical Review E*, **2016**, 93, 032412	2.4	19
44	Machine learning and molecular design of self-assembling -conjugated oligopeptides. *Molecular Simulation*, **2018**, 44, 930-945	2	18
43	Nonlinear machine learning and design of reconfigurable digital colloids. *Soft Matter*, **2016**, 12, 7119-35	3.6	18
42	Molecular Motor Dnm1 Synergistically Induces Membrane Curvature To Facilitate Mitochondrial Fission. *ACS Central Science*, **2017**, 3, 1156-1167	16.8	17
41	Landmark diffusion maps (L-dMaps): Accelerated manifold learning out-of-sample extension. *Applied and Computational Harmonic Analysis*, **2019**, 47, 190-211	3.1	17
40	Nonlinear machine learning in simulations of soft and biological materials. *Molecular Simulation*, **2018**, 44, 1090-1107	2	17
39	Controlling Supramolecular Chirality in Peptide-Peptide Networks by Variation of the Alkyl Spacer Length. *Langmuir*, **2019**, 35, 14060-14073	4	15
38	Computational prediction of broadly neutralizing HIV-1 antibody epitopes from neutralization activity data. *PLoS ONE*, **2013**, 8, e80562	3.7	15
37	Control of the hierarchical assembly of -conjugated optoelectronic peptides by pH and flow. *Organic and Biomolecular Chemistry*, **2017**, 15, 5484-5502	3.9	14
36	Inverse design of self-assembling colloidal crystals with omnidirectional photonic bandgaps. *Soft Matter*, **2019**, 15, 8808-8826	3.6	14
35	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
34	Capabilities and limitations of time-lagged autoencoders for slow mode discovery in dynamical systems. *Journal of Chemical Physics*, **2019**, 151, 064123	3.9	13

33	Molecular latent space simulators. *Chemical Science*, **2020**, 11, 9459-9467	9.4	12
32	Computational design of hepatitis C virus immunogens from host-pathogen dynamics over empirical viral fitness landscapes. *Physical Biology*, **2018**, 16, 016004	3	12
31	Empirical fitness models for hepatitis C virus immunogen design. *Physical Biology*, **2015**, 12, 066006	3	11
30	Accelerated polymerization of N-carboxyanhydrides catalyzed by crown ether. *Nature Communications*, **2021**, 12, 732	17.4	11
29	Patchy Particle Model of the Hierarchical Self-Assembly of π-Conjugated Optoelectronic Peptides. *Journal of Physical Chemistry B*, **2018**, 122, 10219-10236	3.4	11
28	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
27	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
26	MARTINI-Compatible Coarse-Grained Model for the Mesoscale Simulation of Peptoids. *Journal of Physical Chemistry B*, **2020**, 124, 7745-7764	3.4	10
25	Error catastrophe and phase transition in the empirical fitness landscape of HIV. *Physical Review E*, **2015**, 91, 032705	2.4	9
24	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
23	Evidence for Prenucleated Fibrilogenesis of Acid-Mediated Self-Assembling Oligopeptides via Molecular Simulation and Fluorescence Correlation Spectroscopy. *Langmuir*, **2018**, 34, 7346-7354	4	7
22	Global graph matching using diffusion maps. *Intelligent Data Analysis*, **2016**, 20, 637-654	1.1	6
21	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
20	Revealing the Sequence-Structure-Electronic Property Relation of Self-Assembling π-Conjugated Oligopeptides by Molecular and Quantum Mechanical Modeling. *Langmuir*, **2019**, 35, 15221-15231	4	5
19	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
18	Tetranucleosome Interactions Drive Chromatin Folding. *ACS Central Science*, **2021**, 7, 1019-1027	16.8	5
17	100th Anniversary of Macromolecular Science Viewpoint: Data-Driven Protein Design.. *ACS Macro Letters*, **2021**, 10, 327-340	6.6	5
16	Computationally Guided Tuning of Amino Acid Configuration Influences the Chiroptical Properties of Supramolecular Peptide-π-Peptide Nanostructures. *Langmuir*, **2020**, 36, 6782-6792	4	4

15	Near quantitative synthesis of urea macrocycles enabled by bulky N-substituent. *Nature Communications*, **2021**, 12, 1572	17.4	4
14	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
13	Inverse Design of Self-Assembling Diamond Photonic Lattices from Anisotropic Colloidal Clusters. *Journal of Physical Chemistry B*, **2021**, 125, 2398-2410	3.4	3
12	Computationally Guided Tuning of Peptide-Conjugated Perylene Diimide Self-Assembly. *Langmuir*, **2021**, 37, 8594-8606	4	3
11	// Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry B*, **2020**, 124, 9767-9772	3.4	2
10	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
9	Free energy calculations of the functional selectivity of 5-HT2B G protein-coupled receptor. *PLoS ONE*, **2020**, 15, e0243313	3.7	2
8	In search of a novel chassis material for synthetic cells: emergence of synthetic peptide compartment. *Soft Matter*, **2020**, 16, 10769-10780	3.6	2
7	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
6	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
5	// Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry A*, **2020**, 124, 9113-9118	2.8	1
4	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
3	Reconstruction of protein structures from single-molecule time series. *Journal of Chemical Physics*, **2020**, 153, 194102	3.9	1
2	Facile formation of giant elastin-like polypeptide vesicles as synthetic cells. *Chemical Communications*, **2021**, 57, 13202-13205	5.8	1
1	Data-Driven Design and Autonomous Experimentation in Soft and Biological Materials Engineering.. *Annual Review of Chemical and Biomolecular Engineering*, **2022**,	8.9	1