Alpha A Lee

List of Publications by Year
in descending order

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51 papers	3,319 citations	257357 24 h-index	197736 49 g-index
56 all docs	56 docs citations	56 times ranked	3728 citing authors

#	Article	IF	Citations
1	SARS-CoV-2 infects the human kidney and drives fibrosis in kidney organoids. Cell Stem Cell, 2022, 29, 217-231.e8.	5.2	146
2	Expanding the Repertoire of Lowâ€Molecularâ€Weight Pentafluorosulfanylâ€Substituted Scaffolds. ChemMedChem, 2022, 17, e202100641.	1.6	6
3	Impedance-Based Li-Ion Battery Forecasting amid Uneven Usage. ECS Meeting Abstracts, 2022, MA2022-01, 521-521.	0.0	0
4	Data-driven approximations to the bridge function yield improved closures for the Ornsteinâ€“Zernike equation. Soft Matter, 2021, 17, 5393-5400.	1.2	6
5	Discovery of SARS-CoV-2 main protease inhibitors using a synthesis-directed de novo design model. Chemical Communications, 2021, 57, 5909-5912.	2.2	30
6	Quantitative interpretation explains machine learning models for chemical reaction prediction and uncovers bias. Nature Communications, 2021, 12, 1695.	5.8	52
7	Bayesian unsupervised learning reveals hidden structure in concentrated electrolytes. Journal of Chemical Physics, 2021, 154, 134902.	1.2	9
8	Learning the molecular grammar of protein condensates from sequence determinants and embeddings. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	96
9	Modeling the Multiwavelength Variability of Mrk 335 Using Gaussian Processes. Astrophysical Journal, 2021, 914, 144.	1.6	12
10	A white-knuckle ride of open COVID drug discovery. Nature, 2021, 594, 330-332.	13.7	25
11	Predicting the Outcomes of Material Syntheses with Deep Learning. Chemistry of Materials, 2021, 33, 616-624.	3.2	6
12	Mechanistic insight into the chemical treatments of monolayer transition metal disulfides for photoluminescence enhancement. Nature Communications, 2021, 12, 6044.	5.8	17
13	Impact of Chemist-In-The-Loop Molecular Representations on Machine Learning Outcomes. Journal of Chemical Information and Modeling, 2020, 60, 4449-4456.	2.5	9
14	Archetypal landscapes for deep neural networks. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 21857-21864.	3.3	12
15	Predicting materials properties without crystal structure: deep representation learning from stoichiometry. Nature Communications, 2020, 11, 6280.	5.8	147
16	Crowdsourcing drug discovery for pandemics. Nature Chemistry, 2020, 12, 581-581.	6.6	88
17	Geometry of Energy Landscapes and the Optimizability of Deep Neural Networks. Physical Review Letters, 2020, 124, 108301.	2.9	12
18	Fluctuation-induced force in homogeneous isotropic turbulence. Science Advances, 2020, 6, eaba0461.	4.7	4

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19	Validating the validation: reanalyzing a large-scale comparison of deep learning and machine learning models for bioactivity prediction. Journal of Computer-Aided Molecular Design, 2020, 34, 717-730.	1.3	38
20	Identifying degradation patterns of lithium ion batteries from impedance spectroscopy using machine learning. Nature Communications, 2020, 11, 1706.	5.8	263
21	Bayesian semi-supervised learning for uncertainty-calibrated prediction of molecular properties and active learning. Chemical Science, 2019, 10, 8154-8163.	3.7	85
22	Molecular Transformer: A Model for Uncertainty-Calibrated Chemical Reaction Prediction. ACS Central Science, 2019, 5, 1572-1583.	5.3	424
23	Molecular Transformer unifies reaction prediction and retrosynthesis across pharma chemical space. Chemical Communications, 2019, 55, 12152-12155.	2.2	69
24	Ligand biological activity predicted by cleaning positive and negative chemical correlations. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 3373-3378.	3.3	26
25	Controlling Polyelectrolyte Adsorption onto Carbon Nanotubes by Tuning Ionâ€“Image Interactions. Journal of Physical Chemistry B, 2018, 122, 1545-1550.	1.2	4
26	Casimir force in dense confined electrolytes. Molecular Physics, 2018, 116, 3147-3153.	0.8	8
27	Energyâ€“entropy competition and the effectiveness of stochastic gradient descent in machine learning. Molecular Physics, 2018, 116, 3214-3223.	0.8	25
28	Screening Lengths in Ionic Fluids. Physical Review Letters, 2018, 121, 075501.	2.9	37
29	Underscreening in concentrated electrolytes. Faraday Discussions, 2017, 199, 239-259.	1.6	122
30	Switching the Structural Force in Ionic Liquid-Solvent Mixtures by Varying Composition. Physical Review Letters, 2017, 118, 096002.	2.9	68
31	Controlling turbulent drag across electrolytes using electric fields. Faraday Discussions, 2017, 199, 159-173.	1.6	6
32	Long range electrostatic forces in ionic liquids. Chemical Communications, 2017, 53, 1214-1224.	2.2	285
33	Fluctuation spectra and force generation in nonequilibrium systems. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9255-9260.	3.3	12
34	Optimal Design of Experiments by Combining Coarse and Fine Measurements. Physical Review Letters, 2017, 119, 208101.	2.9	5
35	Scaling Analysis of the Screening Length in Concentrated Electrolytes. Physical Review Letters, 2017, 119, 026002.	2.9	163
36	Ionâ€“Image Interactions and Phase Transition at Electrolyteâ€“Metal Interfaces. Journal of Physical Chemistry Letters, 2016, 7, 2753-2757.	2.1	26

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37	The Electrostatic Screening Length in Concentrated Electrolytes Increases with Concentration. Journal of Physical Chemistry Letters, 2016, 7, 2157-2163.	2.1	422
38	Capacitance-Power-Hysteresis Trilemma in Nanoporous Supercapacitors. Physical Review X, 2016, 6, .	2.8	21
39	Microscopic mechanism of thermomolecular orientation and polarization. Soft Matter, 2016, 12, 8661-8665.	1.2	10
40	Predicting proteinâ€“ligand affinity with a random matrix framework. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13564-13569.	3.3	24
41	Quantum capacitance modifies interionic interactions in semiconducting nanopores. Europhysics Letters, 2016, 113, 38005.	0.7	4
42	The role of extensibility in the birth of a ruck in a rug. Extreme Mechanics Letters, 2015, 5, 81-87.	2.0	8
43	Dynamics of Ion Transport in Ionic Liquids. Physical Review Letters, 2015, 115, 106101.	2.9	54
44	Are Room-Temperature Ionic Liquids Dilute Electrolytes?. Journal of Physical Chemistry Letters, 2015, 6, 159-163.	2.1	118
45	Single-File Charge Storage in Conducting Nanopores. Physical Review Letters, 2014, 113, 048701.	2.9	60
46	Charging dynamics of supercapacitors with narrow cylindrical nanopores. Nanotechnology, 2014, 25, 315401.	1.3	41
47	Alternative radical pairs for cryptochrome-based magnetoreception. Journal of the Royal Society Interface, 2014, 11, 20131063.	1.5	113
48	Interionic Interactions in Conducting Nanoconfinement. ChemPhysChem, 2013, 14, 4121-4125.	1.0	39
49	Electroactuation with single charge carrier ionomers: the roles of electrostatic pressure and steric strain. Soft Matter, 2013, 9, 3767.	1.2	21
50	Statics and dynamics of electroactuation with single-charge-carrier ionomers. Journal of Physics Condensed Matter, 2013, 25, 082203.	0.7	8
51	Materials Informatics Reveals Unexplored Structure Space in Cuprate Superconductors. Advanced Functional Materials, 0, , 2104696.	7.8	3