Alpha A Lee

List of Publications by Year
in descending order

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51 papers	3,319 citations	257101 24 h-index	197535 49 g-index
56 all docs	56 docs citations	56 times ranked	3728 citing authors

#	Article	IF	Citations
1	Molecular Transformer: A Model for Uncertainty-Calibrated Chemical Reaction Prediction. ACS Central Science, 2019, 5, 1572-1583.	5.3	424
2	The Electrostatic Screening Length in Concentrated Electrolytes Increases with Concentration. Journal of Physical Chemistry Letters, 2016, 7, 2157-2163.	2.1	422
3	Long range electrostatic forces in ionic liquids. Chemical Communications, 2017, 53, 1214-1224.	2.2	285
4	Identifying degradation patterns of lithium ion batteries from impedance spectroscopy using machine learning. Nature Communications, 2020, 11, 1706.	5.8	263
5	Scaling Analysis of the Screening Length in Concentrated Electrolytes. Physical Review Letters, 2017, 119, 026002.	2.9	163
6	Predicting materials properties without crystal structure: deep representation learning from stoichiometry. Nature Communications, 2020, 11, 6280.	5.8	147
7	SARS-CoV-2 infects the human kidney and drives fibrosis in kidney organoids. Cell Stem Cell, 2022, 29, 217-231.e8.	5.2	146
8	Underscreening in concentrated electrolytes. Faraday Discussions, 2017, 199, 239-259.	1.6	122
9	Are Room-Temperature Ionic Liquids Dilute Electrolytes?. Journal of Physical Chemistry Letters, 2015, 6, 159-163.	2.1	118
10	Alternative radical pairs for cryptochrome-based magnetoreception. Journal of the Royal Society Interface, 2014, 11, 20131063.	1.5	113
11	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
12	Crowdsourcing drug discovery for pandemics. Nature Chemistry, 2020, 12, 581-581.	6.6	88
13	Bayesian semi-supervised learning for uncertainty-calibrated prediction of molecular properties and active learning. Chemical Science, 2019, 10, 8154-8163.	3.7	85
14	Molecular Transformer unifies reaction prediction and retrosynthesis across pharma chemical space. Chemical Communications, 2019, 55, 12152-12155.	2.2	69
15	Switching the Structural Force in Ionic Liquid-Solvent Mixtures by Varying Composition. Physical Review Letters, 2017, 118, 096002.	2.9	68
16	Single-File Charge Storage in Conducting Nanopores. Physical Review Letters, 2014, 113, 048701.	2.9	60
17	Dynamics of Ion Transport in Ionic Liquids. Physical Review Letters, 2015, 115, 106101.	2.9	54
18	Quantitative interpretation explains machine learning models for chemical reaction prediction and uncovers bias. Nature Communications, 2021, 12, 1695.	5.8	52

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19	Charging dynamics of supercapacitors with narrow cylindrical nanopores. Nanotechnology, 2014, 25, 315401.	1.3	41
20	Interionic Interactions in Conducting Nanoconfinement. ChemPhysChem, 2013, 14, 4121-4125.	1.0	39
21	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
22	Screening Lengths in Ionic Fluids. Physical Review Letters, 2018, 121, 075501.	2.9	37
23	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
24	Ionâ€“Image Interactions and Phase Transition at Electrolyteâ€“Metal Interfaces. Journal of Physical Chemistry Letters, 2016, 7, 2753-2757.	2.1	26
25	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
26	Energyâ€“entropy competition and the effectiveness of stochastic gradient descent in machine learning. Molecular Physics, 2018, 116, 3214-3223.	0.8	25
27	A white-knuckle ride of open COVID drug discovery. Nature, 2021, 594, 330-332.	13.7	25
28	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
29	Electroactuation with single charge carrier ionomers: the roles of electrostatic pressure and steric strain. Soft Matter, 2013, 9, 3767.	1.2	21
30	Capacitance-Power-Hysteresis Trilemma in Nanoporous Supercapacitors. Physical Review X, 2016, 6, .	2.8	21
31	Mechanistic insight into the chemical treatments of monolayer transition metal disulfides for photoluminescence enhancement. Nature Communications, 2021, 12, 6044.	5.8	17
32	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
33	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
34	Geometry of Energy Landscapes and the Optimizability of Deep Neural Networks. Physical Review Letters, 2020, 124, 108301.	2.9	12
35	Modeling the Multiwavelength Variability of Mrk 335 Using Gaussian Processes. Astrophysical Journal, 2021, 914, 144.	1.6	12
36	Microscopic mechanism of thermomolecular orientation and polarization. Soft Matter, 2016, 12, 8661-8665.	1.2	10

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37	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
38	Bayesian unsupervised learning reveals hidden structure in concentrated electrolytes. Journal of Chemical Physics, 2021, 154, 134902.	1.2	9
39	Statics and dynamics of electroactuation with single-charge-carrier ionomers. Journal of Physics Condensed Matter, 2013, 25, 082203.	0.7	8
40	The role of extensibility in the birth of a ruck in a rug. Extreme Mechanics Letters, 2015, 5, 81-87.	2.0	8
41	Casimir force in dense confined electrolytes. Molecular Physics, 2018, 116, 3147-3153.	0.8	8
42	Controlling turbulent drag across electrolytes using electric fields. Faraday Discussions, 2017, 199, 159-173.	1.6	6
43	Data-driven approximations to the bridge function yield improved closures for the Ornsteinâ€“Zernike equation. Soft Matter, 2021, 17, 5393-5400.	1.2	6
44	Predicting the Outcomes of Material Syntheses with Deep Learning. Chemistry of Materials, 2021, 33, 616-624.	3.2	6
45	Expanding the Repertoire of Lowâ€Molecularâ€Weight Pentafluorosulfanylâ€Substituted Scaffolds. ChemMedChem, 2022, 17, e202100641.	1.6	6
46	Optimal Design of Experiments by Combining Coarse and Fine Measurements. Physical Review Letters, 2017, 119, 208101.	2.9	5
47	Quantum capacitance modifies interionic interactions in semiconducting nanopores. Europhysics Letters, 2016, 113, 38005.	0.7	4
48	Controlling Polyelectrolyte Adsorption onto Carbon Nanotubes by Tuning Ionâ€“Image Interactions. Journal of Physical Chemistry B, 2018, 122, 1545-1550.	1.2	4
49	Fluctuation-induced force in homogeneous isotropic turbulence. Science Advances, 2020, 6, eaba0461.	4.7	4
50	Materials Informatics Reveals Unexplored Structure Space in Cuprate Superconductors. Advanced Functional Materials, 0, , 2104696.	7.8	3
51	Impedance-Based Li-Ion Battery Forecasting amid Uneven Usage. ECS Meeting Abstracts, 2022, MA2022-01, 521-521.	0.0	0