O Anatole Von Lilienfeld

List of Publications by Year
in descending order

107	12,410	34100 52	28296 105
papers	citations	h-index	g-index

109	109	109	7625
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Non-covalent interactions between molecular dimers (S66) in electric fields. Electronic Structure, 2022, 4, 014005.	2.8	0
2	An orbital-based representation for accurate quantum machine learning. Journal of Chemical Physics, 2022, 156, 114101.	3.0	11
3	Alchemical geometry relaxation. Journal of Chemical Physics, 2022, 156, 184801.	3.0	6
4	Ab initio machine learning of phase space averages. Journal of Chemical Physics, 2022, 157, .	3.0	4
5	An assessment of the structural resolution of various fingerprints commonly used in machine learning. Machine Learning: Science and Technology, 2021, 2, 015018.	5.0	37
6	Machine learning of free energies in chemical compound space using ensemble representations: Reaching experimental uncertainty for solvation. Journal of Chemical Physics, 2021, 154, 134113.	3.0	30
7	Machine learning meets chemical physics. Journal of Chemical Physics, 2021, 154, 160401.	3.0	37
8	Simplifying inverse materials design problems for fixed lattices with alchemical chirality. Science Advances, 2021, 7, .	10.3	6
9	Elucidating an Atmospheric Brown Carbon Speciesâ€”Toward Supplanting Chemical Intuition with Exhaustive Enumeration and Machine Learning. Environmental Science & Technology, 2021, 55, 8447-8457.	10.0	6
10	Machine learning based energy-free structure predictions of molecules, transition states, and solids. Nature Communications, 2021, 12, 4468.	12.8	53
11	Density Functional Geometries and Zero-Point Energies in Ab Initio Thermochemical Treatments of Compounds with First-Row Atoms (H, C, N, O, F). Journal of Chemical Theory and Computation, 2021, 17, 4872-4890.	5.3	22
12	Toward the design of chemical reactions: Machine learning barriers of competing mechanisms in reactant space. Journal of Chemical Physics, 2021, 155, 064105.	3.0	37
13	Ab Initio Machine Learning in Chemical Compound Space. Chemical Reviews, 2021, 121, 10001-10036.	47.7	83
14	Introduction: Machine Learning at the Atomic Scale. Chemical Reviews, 2021, 121, 9719-9721.	47.7	36
15	Conformer-specific polar cycloaddition of dibromobutadiene with trapped propene ions. Nature Communications, 2021, 12, 6047.	12.8	16
16	Rapid and accurate molecular deprotonation energies from quantum alchemy. Physical Chemistry Chemical Physics, 2020, 22, 10519-10525.	2.8	19
17	Machine Learning Models of Vibrating H₂CO: Comparing Reproducing Kernels, FCHL, and PhysNet. Journal of Physical Chemistry A, 2020, 124, 8853-8865.	2.5	24
18	Retrospective on a decade of machine learning for chemical discovery. Nature Communications, 2020, 11, 4895.	12.8	96

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19	Data enhanced Hammett-equation: reaction barriers in chemical space. Chemical Science, 2020, 11, 11859-11868.	7.4	29
20	Effects of perturbation order and basis set on alchemical predictions. Journal of Chemical Physics, 2020, 153, 144118.	3.0	14
21	Quantum machine learning using atom-in-molecule-based fragments selected on the fly. Nature Chemistry, 2020, 12, 945-951.	13.6	112
22	Neural networks and kernel ridge regression for excited states dynamics of CH₂NH 2+ : From single-state to multi-state representations and multi-property machine learning models. Machine Learning: Science and Technology, 2020, 1, 025009.	5.0	47
23	Exploring chemical compound space with quantum-based machine learning. Nature Reviews Chemistry, 2020, 4, 347-358.	30.2	184
24	Quantum-chemistry-aided identification, synthesis and experimental validation of model systems for conformationally controlled reaction studies: separation of the conformers of 2,3-dibromobuta-1,3-diene in the gas phase. Physical Chemistry Chemical Physics, 2020, 22, 13431-13439.	2.8	6
25	Machine learning the computational cost of quantum chemistry. Machine Learning: Science and Technology, 2020, 1, 025002.	5.0	25
26	Noncovalent Quantum Machine Learning Corrections to Density Functionals. Journal of Chemical Theory and Computation, 2020, 16, 2647-2653.	5.3	18
27	Introducing Machine Learning: Science and Technology. Machine Learning: Science and Technology, 2020, 1, 010201.	5.0	10
28	FCHL revisited: Faster and more accurate quantum machine learning. Journal of Chemical Physics, 2020, 152, 044107.	3.0	192
29	Quantum Machine Learning with Response Operators in Chemical Compound Space. Lecture Notes in Physics, 2020, , 155-169.	0.7	3
30	Quantum Machine Learning in Chemistry and Materials. , 2020, , 1883-1909.		7
31	Wasserstein metric for improved quantum machine learning with adjacency matrix representations. Machine Learning: Science and Technology, 2020, 1, 03LT01.	5.0	11
32	Thousands of reactants and transition states for competing E2 and S N 2 reactions. Machine Learning: Science and Technology, 2020, 1, 045026.	5.0	33
33	On the role of gradients for machine learning of molecular energies and forces. Machine Learning: Science and Technology, 2020, 1, 045018.	5.0	63
34	Alchemical perturbation density functional theory. Physical Review Research, 2020, 2, .	3.6	23
35	Atoms in Molecules from Alchemical Perturbation Density Functional Theory. Journal of Physical Chemistry B, 2019, 123, 10073-10082.	2.6	18
36	Operators in quantum machine learning: Response properties in chemical space. Journal of Chemical Physics, 2019, 150, 064105.	3.0	90

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37	Operator Quantum Machine Learning: Navigating the Chemical Space of Response Properties. Chimia, 2019, 73, 1028.	0.6	9
38	Alchemical Normal Modes Unify Chemical Space. Journal of Physical Chemistry Letters, 2019, 10, 30-39.	4.6	23
39	Boosting Quantum Machine Learning Models with a Multilevel Combination Technique: Pople Diagrams Revisited. Journal of Chemical Theory and Computation, 2019, 15, 1546-1559.	5.3	70
40	Constant size descriptors for accurate machine learning models of molecular properties. Journal of Chemical Physics, 2018, 148, 241718.	3.0	88
41	Alchemical and structural distribution based representation for universal quantum machine learning. Journal of Chemical Physics, 2018, 148, 241717.	3.0	272
42	Generalized Density-Functional Tight-Binding Repulsive Potentials from Unsupervised Machine Learning. Journal of Chemical Theory and Computation, 2018, 14, 2341-2352.	5.3	44
43	Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning. Journal of Chemical Physics, 2018, 148, 241706.	3.0	136
44	Quantum Machine Learning im chemischen Raum. Angewandte Chemie, 2018, 130, 4235-4240.	2.0	3
45	Quantum Machine Learning in Chemical Compound Space. Angewandte Chemie - International Edition, 2018, 57, 4164-4169.	13.8	167
46	Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry. Journal of Chemical Physics, 2018, 148, 241401.	3.0	77
47	Torsional Potentials of Glyoxal, Oxalyl Halides, and Their Thiocarbonyl Derivatives: Challenges for Popular Density Functional Approximations. Journal of Chemical Theory and Computation, 2018, 14, 4806-4817.	5.3	10
48	Quantum Machine Learning in Chemistry and Materials. , 2018, , 1-27.		10
49	Machine learning meets volcano plots: computational discovery of cross-coupling catalysts. Chemical Science, 2018, 9, 7069-7077.	7.4	154
50	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Al</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">Ga</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow><… crystals with direct 2 eV band gaps from computational alchemy. Physical Review Materials, 2018, 2, .	2.4	17
51	Genetic Optimization of Training Sets for Improved Machine Learning Models of Molecular Properties. Journal of Physical Chemistry Letters, 2017, 8, 1351-1359.	4.6	54
52	Prediction Errors of Molecular Machine Learning Models Lower than Hybrid DFT Error. Journal of Chemical Theory and Computation, 2017, 13, 5255-5264.	5.3	435
53	Alchemical Predictions for Computational Catalysis: Potential and Limitations. Journal of Physical Chemistry Letters, 2017, 8, 5002-5007.	4.6	48
54	Exploring dissociative water adsorption on isoelectronically BN doped graphene using alchemical derivatives. Journal of Chemical Physics, 2017, 147, 164113.	3.0	25

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55	Tuning dissociation using isoelectronically doped graphene and hexagonal boron nitride: Water and other small molecules. Journal of Chemical Physics, 2016, 144, 154706.	3.0	20
56	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
57	Communication: Understanding molecular representations in machine learning: The role of uniqueness and target similarity. Journal of Chemical Physics, 2016, 145, 161102.	3.0	219
58	Fast and accurate predictions of covalent bonds in chemical space. Journal of Chemical Physics, 2016, 144, 174110.	3.0	36
59	Machine Learning Energies of 2AMillion Elpasolite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:msub><mml:mrow><mml:mi>C</mml:mi></mml:mrow> 135502.	7.8	313
60	Alchemical screening of ionic crystals. Physical Chemistry Chemical Physics, 2016, 18, 31078-31091.	2.8	25
61	Properties and reactivity of nucleic acids relevant to epigenomics, transcriptomics, and therapeutics. Chemical Society Reviews, 2016, 45, 2637-2655.	38.1	34
62	Electronic spectra from TDDFT and machine learning in chemical space. Journal of Chemical Physics, 2015, 143, 084111.	3.0	173
63	Many Molecular Properties from One Kernel in Chemical Space. Chimia, 2015, 69, 182.	0.6	67
64	Crystal structure representations for machine learning models of formation energies. International Journal of Quantum Chemistry, 2015, 115, 1094-1101.	2.0	334
65	Fourier series of atomic radial distribution functions: A molecular fingerprint for machine learning models of quantum chemical properties. International Journal of Quantum Chemistry, 2015, 115, 1084-1093.	2.0	181
66	Transferable Atomic Multipole Machine Learning Models for Small Organic Molecules. Journal of Chemical Theory and Computation, 2015, 11, 3225-3233.	5.3	91
67	Machine Learning Predictions of Molecular Properties: Accurate Many-Body Potentials and Nonlocality in Chemical Space. Journal of Physical Chemistry Letters, 2015, 6, 2326-2331.	4.6	575
68	Machine Learning of Parameters for Accurate Semiempirical Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2120-2125.	5.3	86
69	Big Data Meets Quantum Chemistry Approximations: The Î”-Machine Learning Approach. Journal of Chemical Theory and Computation, 2015, 11, 2087-2096.	5.3	579
70	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. Journal of Chemical Physics, 2015, 142, 181101.	3.0	56
71	Machine Learning for Quantum Mechanical Properties of Atoms in Molecules. Journal of Physical Chemistry Letters, 2015, 6, 3309-3313.	4.6	169
72	Machine learning for many-body physics: The case of the Anderson impurity model. Physical Review B, 2014, 90, .	3.2	113

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73	Water on BN doped benzene: A hard test for exchange-correlation functionals and the impact of exact exchange on weak binding. Journal of Chemical Physics, 2014, 141, 18C530.	3.0	25
74	Toward transferable interatomic van der Waals interactions without electrons: The role of multipole electrostatics and many-body dispersion. Journal of Chemical Physics, 2014, 141, 034101.	3.0	17
75	Modeling electronic quantum transport with machine learning. Physical Review B, 2014, 89, .	3.2	58
76	Application of Diffusion Monte Carlo to Materials Dominated by van der Waals Interactions. Journal of Chemical Theory and Computation, 2014, 10, 3417-3422.	5.3	67
77	Quantum chemistry structures and properties of 134 kilo molecules. Scientific Data, 2014, 1, 140022.	5.3	887
78	Quantum Mechanical Treatment of Variable Molecular Composition: From 'Alchemical' Changes of State Functions to Rational Compound Design. Chimia, 2014, 68, 602.	0.6	13
79	First principles view on chemical compound space: Gaining rigorous atomistic control of molecular properties. International Journal of Quantum Chemistry, 2013, 113, 1676-1689.	2.0	110
80	Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies. Journal of Chemical Theory and Computation, 2013, 9, 3404-3419.	5.3	499
81	Machine learning of molecular electronic properties in chemical compound space. New Journal of Physics, 2013, 15, 095003.	2.9	482
82	Force correcting atom centred potentials for generalised gradient approximated density functional theory: Approaching hybrid functional accuracy for geometries and harmonic frequencies in small chlorofluorocarbons. Molecular Physics, 2013, 111, 2147-2153.	1.7	9
83	RuppetÂal.Reply:. Physical Review Letters, 2012, 109, .	7.8	20
84	Collective many-body van der Waals interactions in molecular systems. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 14791-14795.	7.1	178
85	Fast and Accurate Modeling of Molecular Atomization Energies with Machine Learning. Physical Review Letters, 2012, 108, 058301.	7.8	1,523
86	Toward Quantitative Structureâ€“Property Relationships for Charge Transfer Rates of Polycyclic Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2011, 7, 2549-2555.	5.3	37
87	Path Integral Computation of Quantum Free Energy Differences Due to Alchemical Transformations Involving Mass and Potential. Journal of Chemical Theory and Computation, 2011, 7, 2358-2369.	5.3	36
88	Molten salt eutectics from atomistic simulations. Physical Review E, 2011, 84, 030201.	2.1	13
89	Enol Tautomers of Watsonâ^'Crick Base Pair Models Are Metastable Because of Nuclear Quantum Effects. Journal of the American Chemical Society, 2010, 132, 11510-11515.	13.7	79
90	Alchemical derivatives of reaction energetics. Journal of Chemical Physics, 2010, 133, 084104.	3.0	57

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91	Long range interactions in nanoscale science. Reviews of Modern Physics, 2010, 82, 1887-1944.	45.6	359
92	Two- and three-body interatomic dispersion energy contributions to binding in molecules and solids. Journal of Chemical Physics, 2010, 132, 234109.	3.0	194
93	Molecular Simulation of the Thermal and Transport Properties of Three Alkali Nitrate Salts. Industrial & Engineering Chemistry Research, 2010, 49, 559-571.	3.7	68
94	Ab initio molecular dynamics calculations of ion hydration free energies. Journal of Chemical Physics, 2009, 130, 204507.	3.0	111
95	Accurate ab initio energy gradients in chemical compound space. Journal of Chemical Physics, 2009, 131, 164102.	3.0	57
96	Structure and band gaps of Ga-(V) semiconductors: The challenge of Ga pseudopotentials. Physical Review B, 2008, 77, .	3.2	24
97	Tuning electronic eigenvalues of benzene via doping. Journal of Chemical Physics, 2007, 127, 064305.	3.0	30
98	Library of dispersion-corrected atom-centered potentials for generalized gradient approximation functionals: Elements H, C, N, O, He, Ne, Ar, and Kr. Physical Review B, 2007, 75, .	3.2	157
99	Spectroscopic properties of trichlorofluoromethane CCl3F calculated by density functional theory. Physical Chemistry Chemical Physics, 2007, 9, 5027.	2.8	2
100	Predicting Noncovalent Interactions between Aromatic Biomolecules with London-Dispersion-Corrected DFT. Journal of Physical Chemistry B, 2007, 111, 14346-14354.	2.6	62
101	Alchemical Variations of Intermolecular Energies According to Molecular Grand-Canonical Ensemble Density Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 1083-1090.	5.3	56
102	Weakly Bonded Complexes of Aliphatic and Aromatic Carbon Compounds Described with Dispersion Corrected Density Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 1673-1679.	5.3	66
103	Molecular grand-canonical ensemble density functional theory and exploration of chemical space. Journal of Chemical Physics, 2006, 125, 154104.	3.0	90
104	Adsorption of Ar on graphite using London dispersion forces corrected Kohn-Sham density functional theory. Physical Review B, 2006, 73, .	3.2	43
105	Variational optimization of effective atom centered potentials for molecular properties. Journal of Chemical Physics, 2005, 122, 014113.	3.0	110
106	Variational Particle Number Approach for Rational Compound Design. Physical Review Letters, 2005, 95, 153002.	7.8	112
107	Optimization of Effective Atom Centered Potentials for London Dispersion Forces in Density Functional Theory. Physical Review Letters, 2004, 93, 153004.	7.8	489