O Anatole Von Lilienfeld

List of Publications by Year
in descending order

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107 papers	12,410 citations	34100 52 h-index	28296 105 g-index
109 all docs	109 docs citations	109 times ranked	7625 citing authors

#	Article	IF	Citations
1	Fast and Accurate Modeling of Molecular Atomization Energies with Machine Learning. Physical Review Letters, 2012, 108, 058301.	7.8	1,523
2	Quantum chemistry structures and properties of 134 kilo molecules. Scientific Data, 2014, 1, 140022.	5.3	887
3	Big Data Meets Quantum Chemistry Approximations: The Î”-Machine Learning Approach. Journal of Chemical Theory and Computation, 2015, 11, 2087-2096.	5.3	579
4	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
5	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
6	Optimization of Effective Atom Centered Potentials for London Dispersion Forces in Density Functional Theory. Physical Review Letters, 2004, 93, 153004.	7.8	489
7	Machine learning of molecular electronic properties in chemical compound space. New Journal of Physics, 2013, 15, 095003.	2.9	482
8	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
9	Long range interactions in nanoscale science. Reviews of Modern Physics, 2010, 82, 1887-1944.	45.6	359
10	Crystal structure representations for machine learning models of formation energies. International Journal of Quantum Chemistry, 2015, 115, 1094-1101.	2.0	334
11	Machine Learning Energies of 2ÂMillion 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:mro 135502.	7.8	313
12	Alchemical and structural distribution based representation for universal quantum machine learning. Journal of Chemical Physics, 2018, 148, 241717.	3.0	272
13	Communication: Understanding molecular representations in machine learning: The role of uniqueness and target similarity. Journal of Chemical Physics, 2016, 145, 161102.	3.0	219
14	Two- and three-body interatomic dispersion energy contributions to binding in molecules and solids. Journal of Chemical Physics, 2010, 132, 234109.	3.0	194
15	FCHL revisited: Faster and more accurate quantum machine learning. Journal of Chemical Physics, 2020, 152, 044107.	3.0	192
16	Exploring chemical compound space with quantum-based machine learning. Nature Reviews Chemistry, 2020, 4, 347-358.	30.2	184
17	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
18	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

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19	Electronic spectra from TDDFT and machine learning in chemical space. Journal of Chemical Physics, 2015, 143, 084111.	3.0	173
20	Machine Learning for Quantum Mechanical Properties of Atoms in Molecules. Journal of Physical Chemistry Letters, 2015, 6, 3309-3313.	4.6	169
21	Quantum Machine Learning in Chemical Compound Space. Angewandte Chemie - International Edition, 2018, 57, 4164-4169.	13.8	167
22	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
23	Machine learning meets volcano plots: computational discovery of cross-coupling catalysts. Chemical Science, 2018, 9, 7069-7077.	7.4	154
24	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
25	Machine learning for many-body physics: The case of the Anderson impurity model. Physical Review B, 2014, 90, .	3.2	113
26	Variational Particle Number Approach for Rational Compound Design. Physical Review Letters, 2005, 95, 153002.	7.8	112
27	Quantum machine learning using atom-in-molecule-based fragments selected on the fly. Nature Chemistry, 2020, 12, 945-951.	13.6	112
28	<i>Ab initio</i> molecular dynamics calculations of ion hydration free energies. Journal of Chemical Physics, 2009, 130, 204507.	3.0	111
29	Variational optimization of effective atom centered potentials for molecular properties. Journal of Chemical Physics, 2005, 122, 014113.	3.0	110
30	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
31	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
32	Retrospective on a decade of machine learning for chemical discovery. Nature Communications, 2020, 11, 4895.	12.8	96
33	Transferable Atomic Multipole Machine Learning Models for Small Organic Molecules. Journal of Chemical Theory and Computation, 2015, 11, 3225-3233.	5.3	91
34	Molecular grand-canonical ensemble density functional theory and exploration of chemical space. Journal of Chemical Physics, 2006, 125, 154104.	3.0	90
35	Operators in quantum machine learning: Response properties in chemical space. Journal of Chemical Physics, 2019, 150, 064105.	3.0	90
36	Constant size descriptors for accurate machine learning models of molecular properties. Journal of Chemical Physics, 2018, 148, 241718.	3.0	88

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37	Machine Learning of Parameters for Accurate Semiempirical Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2120-2125.	5.3	86
38	Ab Initio Machine Learning in Chemical Compound Space. Chemical Reviews, 2021, 121, 10001-10036.	47.7	83
39	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
40	Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry. Journal of Chemical Physics, 2018, 148, 241401.	3.0	77
41	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
42	Molecular Simulation of the Thermal and Transport Properties of Three Alkali Nitrate Salts. Industrial & Engineering Chemistry Research, 2010, 49, 559-571.	3.7	68
43	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
44	Many Molecular Properties from One Kernel in Chemical Space. Chimia, 2015, 69, 182.	0.6	67
45	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
46	On the role of gradients for machine learning of molecular energies and forces. Machine Learning: Science and Technology, 2020, 1, 045018.	5.0	63
47	Predicting Noncovalent Interactions between Aromatic Biomolecules with London-Dispersion-Corrected DFT. Journal of Physical Chemistry B, 2007, 111, 14346-14354.	2.6	62
48	Modeling electronic quantum transport with machine learning. Physical Review B, 2014, 89, .	3.2	58
49	Accurate <i>ab initio</i> energy gradients in chemical compound space. Journal of Chemical Physics, 2009, 131, 164102.	3.0	57
50	Alchemical derivatives of reaction energetics. Journal of Chemical Physics, 2010, 133, 084104.	3.0	57
51	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
52	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. Journal of Chemical Physics, 2015, 142, 181101.	3.0	56
53	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
54	Machine learning based energy-free structure predictions of molecules, transition states, and solids. Nature Communications, 2021, 12, 4468.	12.8	53

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55	Alchemical Predictions for Computational Catalysis: Potential and Limitations. Journal of Physical Chemistry Letters, 2017, 8, 5002-5007.	4.6	48
56	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
57	Generalized Density-Functional Tight-Binding Repulsive Potentials from Unsupervised Machine Learning. Journal of Chemical Theory and Computation, 2018, 14, 2341-2352.	5.3	44
58	Adsorption of Ar on graphite using London dispersion forces corrected Kohn-Sham density functional theory. Physical Review B, 2006, 73, .	3.2	43
59	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
60	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
61	Machine learning meets chemical physics. Journal of Chemical Physics, 2021, 154, 160401.	3.0	37
62	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
63	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
64	Fast and accurate predictions of covalent bonds in chemical space. Journal of Chemical Physics, 2016, 144, 174110.	3.0	36
65	Introduction: Machine Learning at the Atomic Scale. Chemical Reviews, 2021, 121, 9719-9721.	47.7	36
66	Properties and reactivity of nucleic acids relevant to epigenomics, transcriptomics, and therapeutics. Chemical Society Reviews, 2016, 45, 2637-2655.	38.1	34
67	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
68	Tuning electronic eigenvalues of benzene via doping. Journal of Chemical Physics, 2007, 127, 064305.	3.0	30
69	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
70	Data enhanced Hammett-equation: reaction barriers in chemical space. Chemical Science, 2020, 11, 11859-11868.	7.4	29
71	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
72	Alchemical screening of ionic crystals. Physical Chemistry Chemical Physics, 2016, 18, 31078-31091.	2.8	25

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73	Exploring dissociative water adsorption on isoelectronically BN doped graphene using alchemical derivatives. Journal of Chemical Physics, 2017, 147, 164113.	3.0	25
74	Machine learning the computational cost of quantum chemistry. Machine Learning: Science and Technology, 2020, 1, 025002.	5.0	25
75	Structure and band gaps of Ga-(V) semiconductors: The challenge of Ga pseudopotentials. Physical Review B, 2008, 77, .	3.2	24
76	Machine Learning Models of Vibrating H₂CO: Comparing Reproducing Kernels, FCHL, and PhysNet. Journal of Physical Chemistry A, 2020, 124, 8853-8865.	2.5	24
77	Alchemical Normal Modes Unify Chemical Space. Journal of Physical Chemistry Letters, 2019, 10, 30-39.	4.6	23
78	Alchemical perturbation density functional theory. Physical Review Research, 2020, 2, .	3.6	23
79	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
80	Rupp<i>etÂal.</i>Reply:. Physical Review Letters, 2012, 109, .	7.8	20
81	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
82	Rapid and accurate molecular deprotonation energies from quantum alchemy. Physical Chemistry Chemical Physics, 2020, 22, 10519-10525.	2.8	19
83	Atoms in Molecules from Alchemical Perturbation Density Functional Theory. Journal of Physical Chemistry B, 2019, 123, 10073-10082.	2.6	18
84	Noncovalent Quantum Machine Learning Corrections to Density Functionals. Journal of Chemical Theory and Computation, 2020, 16, 2647-2653.	5.3	18
85	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
86	<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
87	Conformer-specific polar cycloaddition of dibromobutadiene with trapped propene ions. Nature Communications, 2021, 12, 6047.	12.8	16
88	Effects of perturbation order and basis set on alchemical predictions. Journal of Chemical Physics, 2020, 153, 144118.	3.0	14
89	Molten salt eutectics from atomistic simulations. Physical Review E, 2011, 84, 030201.	2.1	13
90	Quantum Mechanical Treatment of Variable Molecular Composition: From 'Alchemical' Changes of State Functions to Rational Compound Design. Chimia, 2014, 68, 602.	0.6	13

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91	Wasserstein metric for improved quantum machine learning with adjacency matrix representations. Machine Learning: Science and Technology, 2020, 1, 03LT01.	5.0	11
92	An orbital-based representation for accurate quantum machine learning. Journal of Chemical Physics, 2022, 156, 114101.	3.0	11
93	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
94	Quantum Machine Learning in Chemistry and Materials. , 2018, , 1-27.		10
95	Introducing Machine Learning: Science and Technology. Machine Learning: Science and Technology, 2020, 1, 010201.	5.0	10
96	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
97	Operator Quantum Machine Learning: Navigating the Chemical Space of Response Properties. Chimia, 2019, 73, 1028.	0.6	9
98	Quantum Machine Learning in Chemistry and Materials. , 2020, , 1883-1909.		7
99	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
100	Simplifying inverse materials design problems for fixed lattices with alchemical chirality. Science Advances, 2021, 7, .	10.3	6
101	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
102	Alchemical geometry relaxation. Journal of Chemical Physics, 2022, 156, 184801.	3.0	6
103	<i>Ab initio</i> machine learning of phase space averages. Journal of Chemical Physics, 2022, 157, .	3.0	4
104	Quantum Machine Learning im chemischen Raum. Angewandte Chemie, 2018, 130, 4235-4240.	2.0	3
105	Quantum Machine Learning with Response Operators in Chemical Compound Space. Lecture Notes in Physics, 2020, , 155-169.	0.7	3
106	Spectroscopic properties of trichlorofluoromethane CCl3F calculated by density functional theory. Physical Chemistry Chemical Physics, 2007, 9, 5027.	2.8	2
107	Non-covalent interactions between molecular dimers (S66) in electric fields. Electronic Structure, 2022, 4, 014005.	2.8	0