

O Anatole Von Lilienfeld

List of Publications by Year in descending order

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107
papers

12,410
citations

34105

52
h-index

28297

105
g-index

109
all docs

109
docs citations

109
times ranked

7625
citing authors

#	ARTICLE	IF	CITATIONS
19	Electronic spectra from TDDFT and machine learning in chemical space. <i>Journal of Chemical Physics</i> , 2015, 143, 084111.	3.0	173
20	Machine Learning for Quantum Mechanical Properties of Atoms in Molecules. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3309-3313.	4.6	169
21	Quantum Machine Learning in Chemical Compound Space. <i>Angewandte Chemie - International Edition</i> , 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. <i>Physical Review B</i> , 2007, 75, .	3.2	157
23	Machine learning meets volcano plots: computational discovery of cross-coupling catalysts. <i>Chemical Science</i> , 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. <i>Journal of Chemical Physics</i> , 2018, 148, 241706.	3.0	136
25	Machine learning for many-body physics: The case of the Anderson impurity model. <i>Physical Review B</i> , 2014, 90, .	3.2	113
26	Variational Particle Number Approach for Rational Compound Design. <i>Physical Review Letters</i> , 2005, 95, 153002.	7.8	112
27	Quantum machine learning using atom-in-molecule-based fragments selected on the fly. <i>Nature Chemistry</i> , 2020, 12, 945-951.	13.6	112
28	<i>Ab initio</i> molecular dynamics calculations of ion hydration free energies. <i>Journal of Chemical Physics</i> , 2009, 130, 204507.	3.0	111
29	Variational optimization of effective atom centered potentials for molecular properties. <i>Journal of Chemical Physics</i> , 2005, 122, 014113.	3.0	110
30	First principles view on chemical compound space: Gaining rigorous atomistic control of molecular properties. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1676-1689.	2.0	110
31	Blind test of density-functional-based methods on intermolecular interaction energies. <i>Journal of Chemical Physics</i> , 2016, 145, 124105.	3.0	97
32	Retrospective on a decade of machine learning for chemical discovery. <i>Nature Communications</i> , 2020, 11, 4895.	12.8	96
33	Transferable Atomic Multipole Machine Learning Models for Small Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3225-3233.	5.3	91
34	Molecular grand-canonical ensemble density functional theory and exploration of chemical space. <i>Journal of Chemical Physics</i> , 2006, 125, 154104.	3.0	90
35	Operators in quantum machine learning: Response properties in chemical space. <i>Journal of Chemical Physics</i> , 2019, 150, 064105.	3.0	90
36	Constant size descriptors for accurate machine learning models of molecular properties. <i>Journal of Chemical Physics</i> , 2018, 148, 241718.	3.0	88

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37	Machine Learning of Parameters for Accurate Semiempirical Quantum Chemical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2120-2125.	5.3	86
38	Ab Initio Machine Learning in Chemical Compound Space. <i>Chemical Reviews</i> , 2021, 121, 10001-10036.	47.7	83
39	Enol Tautomers of Watson-Crick Base Pair Models Are Metastable Because of Nuclear Quantum Effects. <i>Journal of the American Chemical Society</i> , 2010, 132, 11510-11515.	13.7	79
40	Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry. <i>Journal of Chemical Physics</i> , 2018, 148, 241401.	3.0	77
41	Boosting Quantum Machine Learning Models with a Multilevel Combination Technique: Pople Diagrams Revisited. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1546-1559.	5.3	70
42	Molecular Simulation of the Thermal and Transport Properties of Three Alkali Nitrate Salts. <i>Industrial & Engineering Chemistry Research</i> , 2010, 49, 559-571.	3.7	68
43	Application of Diffusion Monte Carlo to Materials Dominated by van der Waals Interactions. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3417-3422.	5.3	67
44	Many Molecular Properties from One Kernel in Chemical Space. <i>Chimia</i> , 2015, 69, 182.	0.6	67
45	Weakly Bonded Complexes of Aliphatic and Aromatic Carbon Compounds Described with Dispersion Corrected Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1673-1679.	5.3	66
46	On the role of gradients for machine learning of molecular energies and forces. <i>Machine Learning: Science and Technology</i> , 2020, 1, 045018.	5.0	63
47	Predicting Noncovalent Interactions between Aromatic Biomolecules with London-Dispersion-Corrected DFT. <i>Journal of Physical Chemistry B</i> , 2007, 111, 14346-14354.	2.6	62
48	Modeling electronic quantum transport with machine learning. <i>Physical Review B</i> , 2014, 89, .	3.2	58
49	Accurate <i>ab initio</i> energy gradients in chemical compound space. <i>Journal of Chemical Physics</i> , 2009, 131, 164102.	3.0	57
50	Alchemical derivatives of reaction energetics. <i>Journal of Chemical Physics</i> , 2010, 133, 084104.	3.0	57
51	Alchemical Variations of Intermolecular Energies According to Molecular Grand-Canonical Ensemble Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1083-1090.	5.3	56
52	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. <i>Journal of Chemical Physics</i> , 2015, 142, 181101.	3.0	56
53	Genetic Optimization of Training Sets for Improved Machine Learning Models of Molecular Properties. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1351-1359.	4.6	54
54	Machine learning based energy-free structure predictions of molecules, transition states, and solids. <i>Nature Communications</i> , 2021, 12, 4468.	12.8	53

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55	Alchemical Predictions for Computational Catalysis: Potential and Limitations. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5002-5007.	4.6	48
56	Neural networks and kernel ridge regression for excited states dynamics of CH ₂ NH ₂ ⁺ : From single-state to multi-state representations and multi-property machine learning models. <i>Machine Learning: Science and Technology</i> , 2020, 1, 025009.	5.0	47
57	Generalized Density-Functional Tight-Binding Repulsive Potentials from Unsupervised Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2341-2352.	5.3	44
58	Adsorption of Ar on graphite using London dispersion forces corrected Kohn-Sham density functional theory. <i>Physical Review B</i> , 2006, 73, .	3.2	43
59	Toward Quantitative Structure-Property Relationships for Charge Transfer Rates of Polycyclic Aromatic Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2549-2555.	5.3	37
60	An assessment of the structural resolution of various fingerprints commonly used in machine learning. <i>Machine Learning: Science and Technology</i> , 2021, 2, 015018.	5.0	37
61	Machine learning meets chemical physics. <i>Journal of Chemical Physics</i> , 2021, 154, 160401.	3.0	37
62	Toward the design of chemical reactions: Machine learning barriers of competing mechanisms in reactant space. <i>Journal of Chemical Physics</i> , 2021, 155, 064105.	3.0	37
63	Path Integral Computation of Quantum Free Energy Differences Due to Alchemical Transformations Involving Mass and Potential. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2358-2369.	5.3	36
64	Fast and accurate predictions of covalent bonds in chemical space. <i>Journal of Chemical Physics</i> , 2016, 144, 174110.	3.0	36
65	Introduction: Machine Learning at the Atomic Scale. <i>Chemical Reviews</i> , 2021, 121, 9719-9721.	47.7	36
66	Properties and reactivity of nucleic acids relevant to epigenomics, transcriptomics, and therapeutics. <i>Chemical Society Reviews</i> , 2016, 45, 2637-2655.	38.1	34
67	Thousands of reactants and transition states for competing E2 and S _N 2 reactions. <i>Machine Learning: Science and Technology</i> , 2020, 1, 045026.	5.0	33
68	Tuning electronic eigenvalues of benzene via doping. <i>Journal of Chemical Physics</i> , 2007, 127, 064305.	3.0	30
69	Machine learning of free energies in chemical compound space using ensemble representations: Reaching experimental uncertainty for solvation. <i>Journal of Chemical Physics</i> , 2021, 154, 134113.	3.0	30
70	Data enhanced Hammett-equation: reaction barriers in chemical space. <i>Chemical Science</i> , 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. <i>Journal of Chemical Physics</i> , 2014, 141, 18C530.	3.0	25
72	Alchemical screening of ionic crystals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31078-31091.	2.8	25

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73	Exploring dissociative water adsorption on isoelectronically BN doped graphene using alchemical derivatives. <i>Journal of Chemical Physics</i> , 2017, 147, 164113.	3.0	25
74	Machine learning the computational cost of quantum chemistry. <i>Machine Learning: Science and Technology</i> , 2020, 1, 025002.	5.0	25
75	Structure and band gaps of Ga-(V) semiconductors: The challenge of Ga pseudopotentials. <i>Physical Review B</i> , 2008, 77, .	3.2	24
76	Machine Learning Models of Vibrating H ₂ CO: Comparing Reproducing Kernels, FCHL, and PhysNet. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8853-8865.	2.5	24
77	Alchemical Normal Modes Unify Chemical Space. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 30-39.	4.6	23
78	Alchemical perturbation density functional theory. <i>Physical Review Research</i> , 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). <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4872-4890.	5.3	22
80	Ruppert et al. Reply. <i>Physical Review Letters</i> , 2012, 109, .	7.8	20
81	Tuning dissociation using isoelectronically doped graphene and hexagonal boron nitride: Water and other small molecules. <i>Journal of Chemical Physics</i> , 2016, 144, 154706.	3.0	20
82	Rapid and accurate molecular deprotonation energies from quantum alchemy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10519-10525.	2.8	19
83	Atoms in Molecules from Alchemical Perturbation Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10073-10082.	2.6	18
84	Noncovalent Quantum Machine Learning Corrections to Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Journal of Chemical Physics</i> , 2014, 141, 034101.	3.0	17
86	AlGa _x crystals with direct 2 eV band gaps from computational alchemy. <i>Physical Review Materials</i> , 2018, 2, .	2.4	17
87	Conformer-specific polar cycloaddition of dibromobutadiene with trapped propene ions. <i>Nature Communications</i> , 2021, 12, 6047.	12.8	16
88	Effects of perturbation order and basis set on alchemical predictions. <i>Journal of Chemical Physics</i> , 2020, 153, 144118.	3.0	14
89	Molten salt eutectics from atomistic simulations. <i>Physical Review E</i> , 2011, 84, 030201.	2.1	13
90	Quantum Mechanical Treatment of Variable Molecular Composition: From 'Alchemical' Changes of State Functions to Rational Compound Design. <i>Chimia</i> , 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 CCl ₃ F 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