

O Anatole Von Lilienfeld

List of Publications by Year in descending order

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Version: 2024-02-01

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
1	Non-covalent interactions between molecular dimers (S66) in electric fields. <i>Electronic Structure</i> , 2022, 4, 014005.	2.8	0
2	An orbital-based representation for accurate quantum machine learning. <i>Journal of Chemical Physics</i> , 2022, 156, 114101.	3.0	11
3	Alchemical geometry relaxation. <i>Journal of Chemical Physics</i> , 2022, 156, 184801.	3.0	6
4	<i>Ab initio</i> machine learning of phase space averages. <i>Journal of Chemical Physics</i> , 2022, 157, .	3.0	4
5	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
6	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
7	Machine learning meets chemical physics. <i>Journal of Chemical Physics</i> , 2021, 154, 160401.	3.0	37
8	Simplifying inverse materials design problems for fixed lattices with alchemical chirality. <i>Science Advances</i> , 2021, 7, .	10.3	6
9	Elucidating an Atmospheric Brown Carbon Species—Toward Supplanting Chemical Intuition with Exhaustive Enumeration and Machine Learning. <i>Environmental Science & Technology</i> , 2021, 55, 8447-8457.	10.0	6
10	Machine learning based energy-free structure predictions of molecules, transition states, and solids. <i>Nature Communications</i> , 2021, 12, 4468.	12.8	53
11	Density Functional Geometries and Zero-Point Energies in <i>Ab Initio</i> 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
12	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
13	<i>Ab Initio</i> Machine Learning in Chemical Compound Space. <i>Chemical Reviews</i> , 2021, 121, 10001-10036.	47.7	83
14	Introduction: Machine Learning at the Atomic Scale. <i>Chemical Reviews</i> , 2021, 121, 9719-9721.	47.7	36
15	Conformer-specific polar cycloaddition of dibromobutadiene with trapped propene ions. <i>Nature Communications</i> , 2021, 12, 6047.	12.8	16
16	Rapid and accurate molecular deprotonation energies from quantum alchemy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10519-10525.	2.8	19
17	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
18	Retrospective on a decade of machine learning for chemical discovery. <i>Nature Communications</i> , 2020, 11, 4895.	12.8	96

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19	Data enhanced Hammett-equation: reaction barriers in chemical space. <i>Chemical Science</i> , 2020, 11, 11859-11868.	7.4	29
20	Effects of perturbation order and basis set on alchemical predictions. <i>Journal of Chemical Physics</i> , 2020, 153, 144118.	3.0	14
21	Quantum machine learning using atom-in-molecule-based fragments selected on the fly. <i>Nature Chemistry</i> , 2020, 12, 945-951.	13.6	112
22	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
23	Exploring chemical compound space with quantum-based machine learning. <i>Nature Reviews Chemistry</i> , 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. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13431-13439.	2.8	6
25	Machine learning the computational cost of quantum chemistry. <i>Machine Learning: Science and Technology</i> , 2020, 1, 025002.	5.0	25
26	Noncovalent Quantum Machine Learning Corrections to Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2647-2653.	5.3	18
27	Introducing Machine Learning: Science and Technology. <i>Machine Learning: Science and Technology</i> , 2020, 1, 010201.	5.0	10
28	FCHL revisited: Faster and more accurate quantum machine learning. <i>Journal of Chemical Physics</i> , 2020, 152, 044107.	3.0	192
29	Quantum Machine Learning with Response Operators in Chemical Compound Space. <i>Lecture Notes in Physics</i> , 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. <i>Machine Learning: Science and Technology</i> , 2020, 1, 03LT01.	5.0	11
32	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
33	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
34	Alchemical perturbation density functional theory. <i>Physical Review Research</i> , 2020, 2, .	3.6	23
35	Atoms in Molecules from Alchemical Perturbation Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10073-10082.	2.6	18
36	Operators in quantum machine learning: Response properties in chemical space. <i>Journal of Chemical Physics</i> , 2019, 150, 064105.	3.0	90

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37	Operator Quantum Machine Learning: Navigating the Chemical Space of Response Properties. <i>Chimia</i> , 2019, 73, 1028.	0.6	9
38	Alchemical Normal Modes Unify Chemical Space. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 30-39.	4.6	23
39	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
40	Constant size descriptors for accurate machine learning models of molecular properties. <i>Journal of Chemical Physics</i> , 2018, 148, 241718.	3.0	88
41	Alchemical and structural distribution based representation for universal quantum machine learning. <i>Journal of Chemical Physics</i> , 2018, 148, 241717.	3.0	272
42	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
43	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
44	Quantum Machine Learning im chemischen Raum. <i>Angewandte Chemie</i> , 2018, 130, 4235-4240.	2.0	3
45	Quantum Machine Learning in Chemical Compound Space. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 4164-4169.	13.8	167
46	Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry. <i>Journal of Chemical Physics</i> , 2018, 148, 241401.	3.0	77
47	Torsional Potentials of Glyoxal, Oxalyl Halides, and Their Thiocarbonyl Derivatives: Challenges for Popular Density Functional Approximations. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Chemical Science</i> , 2018, 9, 7069-7077.	7.4	154
50	$\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi mathvariant="normal"} \rangle \text{Al} \langle \text{mml:mi} \rangle \text{x} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{Ga} \langle \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 1 \langle \text{mml:mn} \rangle \langle \text{mml:mo} \rangle \hat{\wedge} \langle \text{mml:mo} \rangle \langle \text{mml:mi} \rangle \text{x} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{crystals with direct 2 eV band gaps from computational alchemy. } \langle \text{mml:mi} \rangle \text{Physical Review Materials, 2018, 2, .}$	2.4	17
51	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
52	Prediction Errors of Molecular Machine Learning Models Lower than Hybrid DFT Error. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5255-5264.	5.3	435
53	Alchemical Predictions for Computational Catalysis: Potential and Limitations. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5002-5007.	4.6	48
54	Exploring dissociative water adsorption on isoelectronically BN doped graphene using alchemical derivatives. <i>Journal of Chemical Physics</i> , 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. <i>Journal of Chemical Physics</i> , 2016, 144, 154706.	3.0	20
56	Blind test of density-functional-based methods on intermolecular interaction energies. <i>Journal of Chemical Physics</i> , 2016, 145, 124105.	3.0	97
57	Communication: Understanding molecular representations in machine learning: The role of uniqueness and target similarity. <i>Journal of Chemical Physics</i> , 2016, 145, 161102.	3.0	219
58	Fast and accurate predictions of covalent bonds in chemical space. <i>Journal of Chemical Physics</i> , 2016, 144, 174110.	3.0	36
59	Machine Learning Energies of 2AMillion Epasolite $\langle \text{stretchy}=\text{"false"} \rangle \langle \text{A} \rangle \langle \text{B} \rangle \langle \text{C} \rangle \langle \text{D} \rangle \langle \text{E} \rangle \langle \text{F} \rangle \langle \text{G} \rangle \langle \text{H} \rangle \langle \text{I} \rangle \langle \text{J} \rangle \langle \text{K} \rangle \langle \text{L} \rangle \langle \text{M} \rangle \langle \text{N} \rangle \langle \text{O} \rangle \langle \text{P} \rangle \langle \text{Q} \rangle \langle \text{R} \rangle \langle \text{S} \rangle \langle \text{T} \rangle \langle \text{U} \rangle \langle \text{V} \rangle \langle \text{W} \rangle \langle \text{X} \rangle \langle \text{Y} \rangle \langle \text{Z} \rangle$ 135502.	3.0	110
60	Alchemical screening of ionic crystals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31078-31091.	2.8	25
61	Properties and reactivity of nucleic acids relevant to epigenomics, transcriptomics, and therapeutics. <i>Chemical Society Reviews</i> , 2016, 45, 2637-2655.	38.1	34
62	Electronic spectra from TDDFT and machine learning in chemical space. <i>Journal of Chemical Physics</i> , 2015, 143, 084111.	3.0	173
63	Many Molecular Properties from One Kernel in Chemical Space. <i>Chimia</i> , 2015, 69, 182.	0.6	67
64	Crystal structure representations for machine learning models of formation energies. <i>International Journal of Quantum Chemistry</i> , 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. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1084-1093.	2.0	181
66	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
67	Machine Learning Predictions of Molecular Properties: Accurate Many-Body Potentials and Nonlocality in Chemical Space. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2326-2331.	4.6	575
68	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
69	Big Data Meets Quantum Chemistry Approximations: The $\hat{\rho}$ -Machine Learning Approach. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2087-2096.	5.3	579
70	Communication: Water on hexagonal boron nitride from diffusion Monte Carlo. <i>Journal of Chemical Physics</i> , 2015, 142, 181101.	3.0	56
71	Machine Learning for Quantum Mechanical Properties of Atoms in Molecules. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3309-3313.	4.6	169
72	Machine learning for many-body physics: The case of the Anderson impurity model. <i>Physical Review B</i> , 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. <i>Journal of Chemical Physics</i> , 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. <i>Journal of Chemical Physics</i> , 2014, 141, 034101.	3.0	17
75	Modeling electronic quantum transport with machine learning. <i>Physical Review B</i> , 2014, 89, .	3.2	58
76	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
77	Quantum chemistry structures and properties of 134 kilo molecules. <i>Scientific Data</i> , 2014, 1, 140022.	5.3	887
78	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
79	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
80	Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3404-3419.	5.3	499
81	Machine learning of molecular electronic properties in chemical compound space. <i>New Journal of Physics</i> , 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. <i>Molecular Physics</i> , 2013, 111, 2147-2153.	1.7	9
83	Ruppel et al. Reply. <i>Physical Review Letters</i> , 2012, 109, .	7.8	20
84	Collective many-body van der Waals interactions in molecular systems. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 14791-14795.	7.1	178
85	Fast and Accurate Modeling of Molecular Atomization Energies with Machine Learning. <i>Physical Review Letters</i> , 2012, 108, 058301.	7.8	1,523
86	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
87	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
88	Molten salt eutectics from atomistic simulations. <i>Physical Review E</i> , 2011, 84, 030201.	2.1	13
89	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
90	Alchemical derivatives of reaction energetics. <i>Journal of Chemical Physics</i> , 2010, 133, 084104.	3.0	57

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91	Long range interactions in nanoscale science. <i>Reviews of Modern Physics</i> , 2010, 82, 1887-1944.	45.6	359
92	Two- and three-body interatomic dispersion energy contributions to binding in molecules and solids. <i>Journal of Chemical Physics</i> , 2010, 132, 234109.	3.0	194
93	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
94	<i>Ab initio</i> molecular dynamics calculations of ion hydration free energies. <i>Journal of Chemical Physics</i> , 2009, 130, 204507.	3.0	111
95	Accurate <i>ab initio</i> energy gradients in chemical compound space. <i>Journal of Chemical Physics</i> , 2009, 131, 164102.	3.0	57
96	Structure and band gaps of Ga-(V) semiconductors: The challenge of Ga pseudopotentials. <i>Physical Review B</i> , 2008, 77, .	3.2	24
97	Tuning electronic eigenvalues of benzene via doping. <i>Journal of Chemical Physics</i> , 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. <i>Physical Review B</i> , 2007, 75, .	3.2	157
99	Spectroscopic properties of trichlorofluoromethane CCl ₃ F calculated by density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5027.	2.8	2
100	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
101	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
102	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
103	Molecular grand-canonical ensemble density functional theory and exploration of chemical space. <i>Journal of Chemical Physics</i> , 2006, 125, 154104.	3.0	90
104	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
105	Variational optimization of effective atom centered potentials for molecular properties. <i>Journal of Chemical Physics</i> , 2005, 122, 014113.	3.0	110
106	Variational Particle Number Approach for Rational Compound Design. <i>Physical Review Letters</i> , 2005, 95, 153002.	7.8	112
107	Optimization of Effective Atom Centered Potentials for London Dispersion Forces in Density Functional Theory. <i>Physical Review Letters</i> , 2004, 93, 153004.	7.8	489