Nicholas Lubbers

List of Publications by Year
in descending order

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26 papers	2,017 citations	430874 18 h-index	552781 26 g-index
27 all docs	27 docs citations	27 times ranked	1795 citing authors

#	Article	IF	Citations
1	Less is more: Sampling chemical space with active learning. Journal of Chemical Physics, 2018, 148, 241733.	3.0	426
2	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. Nature Communications, 2019, 10, 2903.	12.8	399
3	Machine Learning Predicts Laboratory Earthquakes. Geophysical Research Letters, 2017, 44, 9276-9282.	4.0	272
4	Hierarchical modeling of molecular energies using a deep neural network. Journal of Chemical Physics, 2018, 148, 241715.	3.0	221
5	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. Scientific Data, 2020, 7, 134.	5.3	104
6	Discovering a Transferable Charge Assignment Model Using Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 4495-4501.	4.6	88
7	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 4687-4698.	5.3	81
8	Automated discovery of a robust interatomic potential for aluminum. Nature Communications, 2021, 12, 1257.	12.8	47
9	Computationally Efficient Multiscale Neural Networks Applied to Fluid Flow in Complex 3D Porous Media. Transport in Porous Media, 2021, 140, 241-272.	2.6	45
10	Earthquake Catalogâ€Based Machine Learning Identification of Laboratory Fault States and the Effects of Magnitude of Completeness. Geophysical Research Letters, 2018, 45, 13,269.	4.0	39
11	The Rise of Neural Networks for Materials and Chemical Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6227-6243.	4.6	39
12	Machine learned HÃ¼ckel theory: Interfacing physics and deep neural networks. Journal of Chemical Physics, 2021, 154, 244108.	3.0	25
13	Modeling Nanoconfinement Effects Using Active Learning. Journal of Physical Chemistry C, 2020, 124, 22200-22211.	3.1	24
14	Graphics Processing Unit-Accelerated Semiempirical Born Oppenheimer Molecular Dynamics Using PyTorch. Journal of Chemical Theory and Computation, 2020, 16, 4951-4962.	5.3	24
15	Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid. Journal of Chemical Physics, 2020, 153, 104502.	3.0	22
16	A multi-dimensional parametric study of variability in multi-phase flow dynamics during geologic CO2 sequestration accelerated with machine learning. Applied Energy, 2021, 287, 116580.	10.1	21
17	A physics-informed and hierarchically regularized data-driven model for predicting fluid flow through porous media. Journal of Computational Physics, 2021, 443, 110526.	3.8	21
18	Machine learning for molecular dynamics with strongly correlated electrons. Physical Review B, 2019, 99, .	3.2	20

#	Article	IF	Citations
19	Deep learning of dynamically responsive chemical Hamiltonians with semiempirical quantum mechanics. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	19
20	On generalized harmonic number sums. Applied Mathematics and Computation, 2010, 217, 689-698.	2.2	17
21	Pairwise Difference Regression: A Machine Learning Meta-algorithm for Improved Prediction and Uncertainty Quantification in Chemical Search. Journal of Chemical Information and Modeling, 2021, 61, 3846-3857.	5.4	17
22	Predicting phosphorescence energies and inferring wavefunction localization with machine learning. Chemical Science, 2021, 12, 10207-10217.	7.4	14
23	Evaluating diffusion and the thermodynamic factor for binary ionic mixtures. Physics of Plasmas, 2020, 27, .	1.9	10
24	Bond order predictions using deep neural networks. Journal of Applied Physics, 2021, 129, .	2.5	8
25	Ex Machina Determination of Structural Correlation Functions. Journal of Physical Chemistry Letters, 2020, 11, 4372-4378.	4.6	7
26	Machine learning of consistent thermodynamic models using automatic differentiation. Physical Review E, 2022, 105, 045301.	2.1	7