

# Nicholas Lubbers

## List of Publications by Year in descending order

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Version: 2024-02-01

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	Machine learning of consistent thermodynamic models using automatic differentiation. <i>Physical Review E</i> , 2022, 105, 045301.	2.1	7
2	Deep learning of dynamically responsive chemical Hamiltonians with semiempirical quantum mechanics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	7.1	19
3	Bond order predictions using deep neural networks. <i>Journal of Applied Physics</i> , 2021, 129, .	2.5	8
4	Automated discovery of a robust interatomic potential for aluminum. <i>Nature Communications</i> , 2021, 12, 1257.	12.8	47
5	A multi-dimensional parametric study of variability in multi-phase flow dynamics during geologic CO <sub>2</sub> sequestration accelerated with machine learning. <i>Applied Energy</i> , 2021, 287, 116580.	10.1	21
6	Computationally Efficient Multiscale Neural Networks Applied to Fluid Flow in Complex 3D Porous Media. <i>Transport in Porous Media</i> , 2021, 140, 241-272.	2.6	45
7	Machine learned Hückel theory: Interfacing physics and deep neural networks. <i>Journal of Chemical Physics</i> , 2021, 154, 244108.	3.0	25
8	The Rise of Neural Networks for Materials and Chemical Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6227-6243.	4.6	39
9	Pairwise Difference Regression: A Machine Learning Meta-algorithm for Improved Prediction and Uncertainty Quantification in Chemical Search. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3846-3857.	5.4	17
10	A physics-informed and hierarchically regularized data-driven model for predicting fluid flow through porous media. <i>Journal of Computational Physics</i> , 2021, 443, 110526.	3.8	21
11	Predicting phosphorescence energies and inferring wavefunction localization with machine learning. <i>Chemical Science</i> , 2021, 12, 10207-10217.	7.4	14
12	Modeling Nanoconfinement Effects Using Active Learning. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22200-22211.	3.1	24
13	Evaluating diffusion and the thermodynamic factor for binary ionic mixtures. <i>Physics of Plasmas</i> , 2020, 27, .	1.9	10
14	Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid. <i>Journal of Chemical Physics</i> , 2020, 153, 104502.	3.0	22
15	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. <i>Scientific Data</i> , 2020, 7, 134.	5.3	104
16	<i>Ex Machina</i> Determination of Structural Correlation Functions. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4372-4378.	4.6	7
17	Graphics Processing Unit-Accelerated Semiempirical Born Oppenheimer Molecular Dynamics Using PyTorch. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4951-4962.	5.3	24
18	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. <i>Nature Communications</i> , 2019, 10, 2903.	12.8	399

#	ARTICLE	IF	CITATIONS
19	Machine learning for molecular dynamics with strongly correlated electrons. <i>Physical Review B</i> , 2019, 99, .	3.2	20
20	Hierarchical modeling of molecular energies using a deep neural network. <i>Journal of Chemical Physics</i> , 2018, 148, 241715.	3.0	221
21	Earthquake Catalog-Based Machine Learning Identification of Laboratory Fault States and the Effects of Magnitude of Completeness. <i>Geophysical Research Letters</i> , 2018, 45, 13,269.	4.0	39
22	Less is more: Sampling chemical space with active learning. <i>Journal of Chemical Physics</i> , 2018, 148, 241733.	3.0	426
23	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4687-4698.	5.3	81
24	Discovering a Transferable Charge Assignment Model Using Machine Learning. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4495-4501.	4.6	88
25	Machine Learning Predicts Laboratory Earthquakes. <i>Geophysical Research Letters</i> , 2017, 44, 9276-9282.	4.0	272
26	On generalized harmonic number sums. <i>Applied Mathematics and Computation</i> , 2010, 217, 689-698.	2.2	17