Linfeng Zhang

List of Publications by Year
in descending order

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48	4,297	218677	223800
papers	citations	26 h-index	46 g-index

48	48	48	2334
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics. Physical Review Letters, 2018, 120, 143001.	7.8	1,006
2	DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics. Computer Physics Communications, 2018, 228, 178-184.	7.5	727
3	Active learning of uniformly accurate interatomic potentials for materials simulation. Physical Review Materials, 2019, 3, .	2.4	299
4	DP-GEN: A concurrent learning platform for the generation of reliable deep learning based potential energy models. Computer Physics Communications, 2020, 253, 107206.	7.5	271
5	Deep Potential: A General Representation of a Many-Body Potential Energy Surface. Communications in Computational Physics, 2018, 23, .	1.7	164
6	DeePCG: Constructing coarse-grained models via deep neural networks. Journal of Chemical Physics, 2018, 149, 034101.	3.0	141
7	Phase Diagram of a Deep Potential Water Model. Physical Review Letters, 2021, 126, 236001.	7.8	140
8	Free energy of proton transfer at the waterâ€“TiO₂ interface from ab initio deep potential molecular dynamics. Chemical Science, 2020, 11, 2335-2341.	7.4	134
9	Signatures of a liquidâ€“liquid transition in an ab initio deep neural network model for water. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26040-26046.	7.1	112
10	Solving many-electron SchrÃ¶dinger equation using deep neural networks. Journal of Computational Physics, 2019, 399, 108929.	3.8	108
11	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. Computer Physics Communications, 2021, 259, 107624.	7.5	100
12	Raman spectrum and polarizability of liquid water from deep neural networks. Physical Chemistry Chemical Physics, 2020, 22, 10592-10602.	2.8	80
13	Pushing the Limit of Molecular Dynamics with Ab Initio Accuracy to 100 Million Atoms with Machine Learning. , 2020, , .		69
14	When do short-range atomistic machine-learning models fall short?. Journal of Chemical Physics, 2021, 154, 034111.	3.0	61
15	Deep potentials for materials science. Materials Futures, 2022, 1, 022601.	8.4	61
16	Deep neural network for the dielectric response of insulators. Physical Review B, 2020, 102, .	3.2	60
17	A deep potential model with long-range electrostatic interactions. Journal of Chemical Physics, 2022, 156, 124107.	3.0	57
18	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	1.7	52

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19	Deep potential generation scheme and simulation protocol for the Li10GeP2S12-type superionic conductors. Journal of Chemical Physics, 2021, 154, 094703.	3.0	49
20	Reinforced dynamics for enhanced sampling in large atomic and molecular systems. Journal of Chemical Physics, 2018, 148, 124113.	3.0	48
21	Ground State Energy Functional with Hartreeâ€“Fock Efficiency and Chemical Accuracy. Journal of Physical Chemistry A, 2020, 124, 7155-7165.	2.5	42
22	DeePKS: A Comprehensive Data-Driven Approach toward Chemically Accurate Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 170-181.	5.3	40
23	Modeling Liquid Water by Climbing up Jacobâ€™s Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. Journal of Physical Chemistry B, 2021, 125, 11444-11456.	2.6	40
24	Deep learning of accurate force field of ferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>HfO</mml:mi></mml:mrow><mml:mn>2</m Physical Review B, 2021, 103, .	3.2	39
25	Deep learning inter-atomic potential model for accurate irradiation damage simulations. Applied Physics Letters, 2019, 114, .	3.3	31
26	Heat transport in liquid water from first-principles and deep neural network simulations. Physical Review B, 2021, 104, .	3.2	29
27	Specialising neural network potentials for accurate properties and application to the mechanical response of titanium. Npj Computational Materials, 2021, 7, .	8.7	26
28	Accurate Deep Potential model for the Alâ€“Cuâ€“Mg alloy in the full concentration space*. Chinese Physics B, 2021, 30, 050706.	1.4	25
29	Structural phase transitions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> from deep potential molecular dynamics. Physical Review B, 2022, 105, .	3.2	25
30	Viscosity in water from first-principles and deep-neural-network simulations. Npj Computational Materials, 2022, 8, .	8.7	23
31	Exploring the Chemical Space of Linear Alkane Pyrolysis via Deep Potential GENerator. Energy & Fuels, 2021, 35, 762-769.	5.1	22
32	Isotope effects in molecular structures and electronic properties of liquid water via deep potential molecular dynamics based on the SCAN functional. Physical Review B, 2020, 102, .	3.2	22
33	The chemical origin of temperature-dependent lithium-ion concerted diffusion in sulfide solid electrolyte Li10GeP2S12. Journal of Energy Chemistry, 2022, 70, 59-66.	12.9	22
34	Warm dense matter simulation via electron temperature dependent deep potential molecular dynamics. Physics of Plasmas, 2020, 27, .	1.9	19
35	Combined Deep Learning and Classical Potential Approach for Modeling Diffusion in UiO-66. Journal of Chemical Theory and Computation, 2022, 18, 3593-3606.	5.3	19
36	Efficiently Trained Deep Learning Potential for Graphane. Journal of Physical Chemistry C, 2021, 125, 14874-14882.	3.1	18

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37	Efficient sampling of high-dimensional free energy landscapes using adaptive reinforced dynamics. Nature Computational Science, 2022, 2, 20-29.	8.0	18
38	Neural Canonical Transformation with Symplectic Flows. Physical Review X, 2020, 10, .	8.9	13
39	Adaptive coupling of a deep neural network potential to a classical force field. Journal of Chemical Physics, 2018, 149, 154107.	3.0	11
40	Crystal Structure Prediction of Binary Alloys via Deep Potential. Frontiers in Chemistry, 2020, 8, 589795.	3.6	11
41	Machine-learning-assisted modeling. Physics Today, 2021, 74, 36-41.	0.3	11
42	Deep Density: Circumventing the Kohn-Sham equations via symmetry preserving neural networks. Journal of Computational Physics, 2021, 443, 110523.	3.8	11
43	Machine learning phase space quantum dynamics approaches. Journal of Chemical Physics, 2021, 154, 184104.	3.0	10
44	Extending the limit of molecular dynamics with ab initio accuracy to 10 billion atoms. , 2022, , .		8
45	A generalizable machine learning potential of Agâ€“Au nanoalloys and its application to surface reconstruction, segregation and diffusion. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 025003.	2.0	8
46	Isotope effects in x-ray absorption spectra of liquid water. Physical Review B, 2020, 102, .	3.2	6
47	Neural network representation of electronic structure from ab initio molecular dynamics. Science Bulletin, 2022, 67, 29-37.	9.0	5
48	Universal approximation of symmetric and anti-symmetric functions. Communications in Mathematical Sciences, 2022, 20, 1397-1408.	1.0	4