Han Wang

List of Publications by Year
in descending order

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		201674	155660
58	4,308	27	55
papers	citations	h-index	g-index

58	58	58	2733
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	Comparative atomistic and coarse-grained study of water: What do we lose by coarse-graining?. European Physical Journal E, 2009, 28, 221-229.	1.6	231
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	Optimizing working parameters of the smooth particle mesh Ewald algorithm in terms of accuracy and efficiency. Journal of Chemical Physics, 2010, 133, 034117.	3.0	108
9	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. Computer Physics Communications, 2021, 259, 107624.	7.5	100
10	Raman spectrum and polarizability of liquid water from deep neural networks. Physical Chemistry Chemical Physics, 2020, 22, 10592-10602.	2.8	80
11	Pushing the Limit of Molecular Dynamics with Ab Initio Accuracy to 100 Million Atoms with Machine Learning. , 2020, , .		69
12	Deep potentials for materials science. Materials Futures, 2022, 1, 022601.	8.4	61
13	Deep neural network for the dielectric response of insulators. Physical Review B, 2020, 102, .	3.2	60
14	A deep potential model with long-range electrostatic interactions. Journal of Chemical Physics, 2022, 156, 124107.	3.0	57
15	Adaptive Resolution Simulation (AdResS): A Smooth Thermodynamic and Structural Transition from Atomistic to Coarse Grained Resolution and Vice Versa in a Grand Canonical Fashion. Journal of Chemical Theory and Computation, 2012, 8, 2878-2887.	5.3	56
16	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	1.7	52
17	Grand-Canonical-like Molecular-Dynamics Simulations by Using an Adaptive-Resolution Technique. Physical Review X, 2013, 3, .	8.9	51
18	Molecular dynamics in a grand ensemble: Bergmannâ€“Lebowitz model and adaptive resolution simulation. New Journal of Physics, 2015, 17, 083042.	2.9	49

#	Article	IF	Citations
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	Chemical potential of liquids and mixtures via adaptive resolution simulation. Journal of Chemical Physics, 2014, 141, 034102.	3.0	47
22	Ground State Energy Functional with Hartreeâ€“Fock Efficiency and Chemical Accuracy. Journal of Physical Chemistry A, 2020, 124, 7155-7165.	2.5	42
23	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
24	Applications of the Cross-Entropy Method to Importance Sampling and Optimal Control of Diffusions. SIAM Journal of Scientific Computing, 2014, 36, A2654-A2672.	2.8	39
25	Multiple Staggered Mesh Ewald: Boosting the Accuracy of the Smooth Particle Mesh Ewald Method. Journal of Chemical Theory and Computation, 2016, 12, 5596-5608.	5.3	32
26	Deep learning inter-atomic potential model for accurate irradiation damage simulations. Applied Physics Letters, 2019, 114, .	3.3	31
27	Determining hydrodynamic boundary conditions from equilibrium fluctuations. Physical Review E, 2015, 92, 043007.	2.1	29
28	Heat transport in liquid water from first-principles and deep neural network simulations. Physical Review B, 2021, 104, .	3.2	29
29	Specialising neural network potentials for accurate properties and application to the mechanical response of titanium. Npj Computational Materials, 2021, 7, .	8.7	26
30	A critical appraisal of the zero-multipole method: Structural, thermodynamic, dielectric, and dynamical properties of a water system. Journal of Chemical Physics, 2016, 144, 114503.	3.0	23
31	Exploring the Chemical Space of Linear Alkane Pyrolysis via Deep Potential GENerator. Energy & Fuels, 2021, 35, 762-769.	5.1	22
32	An efficient adaptive mesh redistribution method for a non-linear Dirac equation. Journal of Computational Physics, 2007, 222, 176-193.	3.8	21
33	Building Markov State Models for Periodically Driven Non-Equilibrium Systems. Journal of Chemical Theory and Computation, 2015, 11, 1819-1831.	5.3	20
34	Crucial properties of the moment closure model FENE-QE. Journal of Non-Newtonian Fluid Mechanics, 2008, 150, 80-92.	2.4	19
35	Warm dense matter simulation via electron temperature dependent deep potential molecular dynamics. Physics of Plasmas, 2020, 27, .	1.9	19
36	Adaptive resolution simulation in equilibrium and beyond. European Physical Journal: Special Topics, 2015, 224, 2269-2287.	2.6	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	Exploring the Conformational Dynamics of Alanine Dipeptide in Solution Subjected to an External Electric Field: A Nonequilibrium Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2014, 10, 1376-1386.	5.3	17
39	Sampling the isothermal-isobaric ensemble by Langevin dynamics. Journal of Chemical Physics, 2016, 144, 124113.	3.0	14
40	Applicability of Kerker preconditioning scheme to the self-consistent density functional theory calculations of inhomogeneous systems. Physical Review E, 2018, 97, 033305.	2.1	14
41	Ab initio validation on the connection between atomistic and hydrodynamic description to unravel the ion dynamics of warm dense matter. Physical Review Research, 2021, 3, .	3.6	14
42	On the existence of the optimal order for wavefunction extrapolation in Born-Oppenheimer molecular dynamics. Journal of Chemical Physics, 2016, 144, 244103.	3.0	12
43	On the Numerical Accuracy of Ewald, Smooth Particle Mesh Ewald, and Staggered Mesh Ewald Methods for Correlated Molecular Systems. Journal of Chemical Theory and Computation, 2012, 8, 3243-3256.	5.3	11
44	Adaptive coupling of a deep neural network potential to a classical force field. Journal of Chemical Physics, 2018, 149, 154107.	3.0	11
45	Crystal Structure Prediction of Binary Alloys via Deep Potential. Frontiers in Chemistry, 2020, 8, 589795.	3.6	11
46	Measuring the Spontaneous Curvature of Bilayer Membranes by Molecular Dynamics Simulations. Communications in Computational Physics, 2013, 13, 1093-1106.	1.7	10
47	Toward accurate electronic, optical, and vibrational properties of hexagonal Si, Ge, and Si1â^'xGex alloys from first-principle simulations. Journal of Applied Physics, 2021, 129, .	2.5	10
48	Error estimate of short-range force calculation in inhomogeneous molecular systems. Physical Review E, 2012, 86, 026704.	2.1	9
49	Extending the limit of molecular dynamics with ab initio accuracy to 10 billion atoms. , 2022, , .		8
50	Parallel 3-dim fast Fourier transforms with load balancing of the plane waves. Computer Physics Communications, 2017, 211, 54-60.	7.5	7
51	On the existence of a third-order phase transition beyond the Andrews critical point: A molecular dynamics study. Journal of Chemical Physics, 2011, 135, 224506.	3.0	6
52	Deep-learning potential method to simulate shear viscosity of liquid aluminum at high temperature and high pressure by molecular dynamics. AIP Advances, 2021, 11, .	1.3	6
53	The optimal particle-mesh interpolation basis. Journal of Chemical Physics, 2017, 147, 124107.	3.0	5
54	Biot's equations-based reservoir parameter inversion using deep neural networks. Journal of Geophysics and Engineering, 2021, 18, 862-874.	1.4	5

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55	Linear response theory and optimal control for a molecular system under non-equilibriumÂconditions. Molecular Physics, 2013, 111, 3555-3564.	1.7	4
56	Kaiser-Bessel basis for particle-mesh interpolation. Physical Review E, 2017, 95, 063303.	2.1	3
57	Is there a third order phase transition for supercritical fluids?. Journal of Chemical Physics, 2014, 140, 014502.	3.0	1
58	Reply to comment by R. Klein on â€œAdaptive resolution simulation in equilibrium and beyondâ€• European Physical Journal: Special Topics, 2015, 224, 2501-2502.	2.6	0