JÃ¶rg Behler

List of Publications by Year
in descending order

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112	14,701	26567	22764
papers	citations	56 h-index	112 g-index

119	119	119	7094
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Neural Network Potentials: A Concise Overview of Methods. Annual Review of Physical Chemistry, 2022, 73, 163-186.	4.8	69
2	A Hessian-based assessment of atomic forces for training machine learning interatomic potentials. Journal of Chemical Physics, 2022, 156, 114106.	1.2	6
3	A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer. Nature Communications, 2021, 12, 398.	5.8	215
4	An assessment of the structural resolution of various fingerprints commonly used in machine learning. Machine Learning: Science and Technology, 2021, 2, 015018.	2.4	37
5	Four Generations of High-Dimensional Neural Network Potentials. Chemical Reviews, 2021, 121, 10037-10072.	23.0	292
6	A bin and hash method for analyzing reference data and descriptors in machine learning potentials. Machine Learning: Science and Technology, 2021, 2, 037001.	2.4	2
7	Properties of Î±-Brass Nanoparticles II: Structure and Composition. Journal of Physical Chemistry C, 2021, 125, 14897-14909.	1.5	9
8	Machine learning potentials for extended systems: a perspective. European Physical Journal B, 2021, 94, 1.	0.6	81
9	General-Purpose Machine Learning Potentials Capturing Nonlocal Charge Transfer. Accounts of Chemical Research, 2021, 54, 808-817.	7.6	65
10	Mechanism of amorphous phase stabilization in ultrathin films of monoatomic phase change material. Nanoscale, 2021, 13, 16146-16155.	2.8	22
11	High-dimensional neural network potentials for magnetic systems using spin-dependent atom-centered symmetry functions. Npj Computational Materials, 2021, 7, .	3.5	30
12	Insights into lithium manganese oxideâ€“water interfaces using machine learning potentials. Journal of Chemical Physics, 2021, 155, 244703.	1.2	18
13	Temperature dependence of the vibrational spectrum of porphycene: a qualitative failure of classical-nuclei molecular dynamics. Faraday Discussions, 2020, 221, 526-546.	1.6	22
14	Temperature effects on the ionic conductivity in concentrated alkaline electrolyte solutions. Physical Chemistry Chemical Physics, 2020, 22, 10426-10430.	1.3	25
15	Atomistic simulations of thermal conductivity in GeTe nanowires. Journal Physics D: Applied Physics, 2020, 53, 054001.	1.3	20
16	Automated Fitting of Neural Network Potentials at Coupled Cluster Accuracy: Protonated Water Clusters as Testing Ground. Journal of Chemical Theory and Computation, 2020, 16, 88-99.	2.3	80
17	Transferability of neural network potentials for varying stoichiometry: Phonons and thermal conductivity of MnxGey compounds. Journal of Applied Physics, 2020, 127, .	1.1	27
18	Global optimization of copper clusters at the ZnO(101Â¯0) surface using a DFT-based neural network potential and genetic algorithms. Journal of Chemical Physics, 2020, 153, 054704.	1.2	33

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19	Insights into Water Permeation through hBN Nanocapillaries by Ab Initio Machine Learning Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2020, 11, 7363-7370.	2.1	33
20	Closing the gap between theory and experiment for lithium manganese oxide spinels using a high-dimensional neural network potential. Physical Review B, 2020, 102, .	1.1	24
21	Predicting oxidation and spin states by high-dimensional neural networks: Applications to lithium manganese oxide spinels. Journal of Chemical Physics, 2020, 153, 164107.	1.2	26
22	An experimentally validated neural-network potential energy surface for H-atom on free-standing graphene in full dimensionality. Physical Chemistry Chemical Physics, 2020, 22, 26113-26120.	1.3	14
23	Hybrid density functional theory benchmark study on lithium manganese oxides. Physical Review B, 2020, 101, .	1.1	12
24	Accurate Global Potential Energy Surfaces for the H + CH₃OH Reaction by Neural Network Fitting with Permutation Invariance. Journal of Physical Chemistry A, 2020, 124, 5737-5745.	1.1	40
25	A flexible and adaptive grid algorithm for global optimization utilizing basin hopping Monte Carlo. Journal of Chemical Physics, 2020, 152, 094109.	1.2	6
26	Performance and Cost Assessment of Machine Learning Interatomic Potentials. Journal of Physical Chemistry A, 2020, 124, 731-745.	1.1	428
27	Properties of Î±-Brass Nanoparticles. 1. Neural Network Potential Energy Surface. Journal of Physical Chemistry C, 2020, 124, 12682-12695.	1.5	27
28	Neural Network Potentials in Materials Modeling. , 2020, , 661-680.		4
29	High-Dimensional Neural Network Potentials for Atomistic Simulations. Lecture Notes in Physics, 2020, , 253-275.	0.3	1
30	New Insights into the Catalytic Activity of Cobalt Orthophosphate Co 3 (PO 4) 2 from Charge Density Analysis. Chemistry - A European Journal, 2019, 25, 15786-15794.	1.7	4
31	Priming effects in the crystallization of the phase change compound GeTe from atomistic simulations. Faraday Discussions, 2019, 213, 287-301.	1.6	18
32	One-dimensional vs. two-dimensional proton transport processes at solidâ€“liquid zinc-oxideâ€“water interfaces. Chemical Science, 2019, 10, 1232-1243.	3.7	39
33	Library-Based LAMMPS Implementation of High-Dimensional Neural Network Potentials. Journal of Chemical Theory and Computation, 2019, 15, 1827-1840.	2.3	175
34	A critical comparison of neural network potentials for molecular reaction dynamics with exact permutation symmetry. Physical Chemistry Chemical Physics, 2019, 21, 9672-9682.	1.3	39
35	From Molecular Fragments to the Bulk: Development of a Neural Network Potential for MOF-5. Journal of Chemical Theory and Computation, 2019, 15, 3793-3809.	2.3	72
36	Orbital-Dependent Electronic Friction Significantly Affects the Description of Reactive Scattering of N₂ from Ru(0001). Journal of Physical Chemistry Letters, 2019, 10, 2957-2962.	2.1	45

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37	Parallel Multistream Training of High-Dimensional Neural Network Potentials. Journal of Chemical Theory and Computation, 2019, 15, 3075-3092.	2.3	124
38	Accurate Probabilities for Highly Activated Reaction of Polyatomic Molecules on Surfaces Using a High-Dimensional Neural Network Potential: CHD₃ + Cu(111). Journal of Physical Chemistry Letters, 2019, 10, 1763-1768.	2.1	56
39	High-Dimensional Neural Network Potentials for Atomistic Simulations. ACS Symposium Series, 2019, , 49-59.	0.5	2
40	Structure and Dynamics of the Liquidâ€“Water/Zinc-Oxide Interface from Machine Learning Potential Simulations. Journal of Physical Chemistry C, 2019, 123, 1293-1304.	1.5	58
41	Ab initio thermodynamics of liquid and solid water. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 1110-1115.	3.3	201
42	Comparison of permutationally invariant polynomials, neural networks, and Gaussian approximation potentials in representing water interactions through many-body expansions. Journal of Chemical Physics, 2018, 148, 241725.	1.2	142
43	Maximally resolved anharmonic OH vibrational spectrum of the water/ZnO(101Â¯0) interface from a high-dimensional neural network potential. Journal of Chemical Physics, 2018, 148, 241720.	1.2	28
44	High-dimensional neural network potentials for solvation: The case of protonated water clusters in helium. Journal of Chemical Physics, 2018, 148, 102310.	1.2	30
45	Analysis of Energy Dissipation Channels in a Benchmark System of Activated Dissociation: N₂ on Ru(0001). Journal of Physical Chemistry C, 2018, 122, 23470-23480.	1.5	15
46	Nuclear Quantum Effects in Sodium Hydroxide Solutions from Neural Network Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 10158-10171.	1.2	29
47	Neural Network Potentials in Materials Modeling. , 2018, , 1-20.		7
48	Density anomaly of water at negative pressures from first principles. Journal of Physics Condensed Matter, 2018, 30, 254005.	0.7	10
49	Automatic selection of atomic fingerprints and reference configurations for machine-learning potentials. Journal of Chemical Physics, 2018, 148, 241730.	1.2	224
50	Self-Diffusion of Surface Defects at Copperâ€“Water Interfaces. Journal of Physical Chemistry C, 2017, 121, 4368-4383.	1.5	31
51	Accurate Neural Network Description of Surface Phonons in Reactive Gasâ€“Surface Dynamics: N₂ + Ru(0001). Journal of Physical Chemistry Letters, 2017, 8, 2131-2136.	2.1	126
52	First Principles Neural Network Potentials for Reactive Simulations of Large Molecular and Condensed Systems. Angewandte Chemie - International Edition, 2017, 56, 12828-12840.	7.2	462
53	Hochdimensionale neuronale Netze fÃ¼r Potentialhyperflächen groÃŸer molekularer und kondensierter Systeme. Angewandte Chemie, 2017, 129, 13006-13020.	1.6	17
54	Proton-Transfer-Driven Water Exchange Mechanism in the Na+ Solvation Shell. Journal of Physical Chemistry B, 2017, 121, 4184-4190.	1.2	18

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55	Proton-Transfer Mechanisms at the Waterâ€“ZnO Interface: The Role of Presolvation. Journal of Physical Chemistry Letters, 2017, 8, 1476-1483.	2.1	106
56	Surface phase diagram prediction from a minimal number of DFT calculations: redox-active adsorbates on zinc oxide. Physical Chemistry Chemical Physics, 2017, 19, 28731-28748.	1.3	4
57	Atomistic Simulations of the Crystallization and Aging of GeTe Nanowires. Journal of Physical Chemistry C, 2017, 121, 23827-23838.	1.5	42
58	Machine learning molecular dynamics for the simulation of infrared spectra. Chemical Science, 2017, 8, 6924-6935.	3.7	349
59	Structure of aqueous NaOH solutions: insights from neural-network-based molecular dynamics simulations. Physical Chemistry Chemical Physics, 2017, 19, 82-96.	1.3	64
60	How van der Waals interactions determine the unique properties of water. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8368-8373.	3.3	312
61	Atomic mobility in the overheated amorphous GeTe compound for phase change memories. Physica Status Solidi (A) Applications and Materials Science, 2016, 213, 329-334.	0.8	9
62	High order path integrals made easy. Journal of Chemical Physics, 2016, 145, 234103.	1.2	47
63	Perspective: Machine learning potentials for atomistic simulations. Journal of Chemical Physics, 2016, 145, 170901.	1.2	879
64	Comparing the accuracy of high-dimensional neural network potentials and the systematic molecular fragmentation method: A benchmark study for all-trans alkanes. Journal of Chemical Physics, 2016, 144, 194110.	1.2	48
65	Nuclear Quantum Effects in Water at the Triple Point: Using Theory as a Link Between Experiments. Journal of Physical Chemistry Letters, 2016, 7, 2210-2215.	2.1	57
66	Neural network molecular dynamics simulations of solidâ€“liquid interfaces: water at low-index copper surfaces. Physical Chemistry Chemical Physics, 2016, 18, 28704-28725.	1.3	141
67	Mode specific dynamics in the H2 + SH â† H + H2S reaction. Physical Chemistry Chemical Physics, 2016, 18, 29113-29121.	1.3	21
68	Concentration-Dependent Proton Transfer Mechanisms in Aqueous NaOH Solutions: From Acceptor-Driven to Donor-Driven and Back. Journal of Physical Chemistry Letters, 2016, 7, 3302-3306.	2.1	66
69	Peeling by Nanomechanical Forces: A Route to Selective Creation of Surface Structures. Physical Review Letters, 2015, 115, 036102.	2.9	10
70	Constructing highâ€dimensional neural network potentials: A tutorial review. International Journal of Quantum Chemistry, 2015, 115, 1032-1050.	1.0	569
71	Electron-phonon interaction and thermal boundary resistance at the crystal-amorphous interface of the phase change compound GeTe. Journal of Applied Physics, 2015, 117, .	1.1	41
72	Heterogeneous Crystallization of the Phase Change Material GeTe via Atomistic Simulations. Journal of Physical Chemistry C, 2015, 119, 6428-6434.	1.5	28

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73	Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. Physical Review B, 2015, 92, .	1.1	82
74	Representing the potential-energy surface of protonated water clusters by high-dimensional neural network potentials. Physical Chemistry Chemical Physics, 2015, 17, 8356-8371.	1.3	69
75	Dynamical Heterogeneity in the Supercooled Liquid State of the Phase Change Material GeTe. Journal of Physical Chemistry B, 2014, 118, 13621-13628.	1.2	57
76	Representing potential energy surfaces by high-dimensional neural network potentials. Journal of Physics Condensed Matter, 2014, 26, 183001.	0.7	252
77	Next generation interatomic potentials for condensed systems. European Physical Journal B, 2014, 87, 1.	0.6	65
78	Force-induced mechanical response of moleculeâ€“metal interfaces: molecular nanomechanics of propanethiolate self-assembled monolayers on Au(111). Physical Chemistry Chemical Physics, 2013, 15, 16001.	1.3	13
79	A Full-Dimensional Neural Network Potential-Energy Surface for Water Clusters up to the Hexamer. Zeitschrift Fur Physikalische Chemie, 2013, 227, .	1.4	25
80	Fast Crystallization of the Phase Change Compound GeTe by Large-Scale Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2013, 4, 4241-4246.	2.1	133
81	Adsorption of Methanethiolate and Atomic Sulfur at the Cu(111) Surface: A Computational Study. Journal of Physical Chemistry C, 2013, 117, 337-348.	1.5	11
82	A Density-Functional Theory-Based Neural Network Potential for Water Clusters Including van der Waals Corrections. Journal of Physical Chemistry A, 2013, 117, 7356-7366.	1.1	157
83	Neural network potentials for metals and oxides â€“ First applications to copper clusters at zinc oxide. Physica Status Solidi (B): Basic Research, 2013, 250, 1191-1203.	0.7	113
84	Construction of high-dimensional neural network potentials using environment-dependent atom pairs. Journal of Chemical Physics, 2012, 136, 194111.	1.2	107
85	A neural network potential-energy surface for the water dimer based on environment-dependent atomic energies and charges. Journal of Chemical Physics, 2012, 136, 064103.	1.2	117
86	Thermal transport in phase-change materials from atomistic simulations. Physical Review B, 2012, 86, .	1.1	75
87	Neural network interatomic potential for the phase change material GeTe. Physical Review B, 2012, 85, .	1.1	198
88	High-dimensional neural network potentials for metal surfaces: A prototype study for copper. Physical Review B, 2012, 85, .	1.1	249
89	Breakdown of Stokesâ€“Einstein relation in the supercooled liquid state of phase change materials. Physica Status Solidi (B): Basic Research, 2012, 249, 1880-1885.	0.7	75
90	Microscopic Origins of the Anomalous Melting Behavior of Sodium under High Pressure. Physical Review Letters, 2012, 108, 115701.	2.9	64

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91	Neural network potential-energy surfaces in chemistry: a tool for large-scale simulations. Physical Chemistry Chemical Physics, 2011, 13, 17930.	1.3	573
92	Atom-centered symmetry functions for constructing high-dimensional neural network potentials. Journal of Chemical Physics, 2011, 134, 074106.	1.2	1,014
93	High-dimensional neural-network potentials for multicomponent systems: Applications to zinc oxide. Physical Review B, 2011, 83, .	1.1	286
94	Nucleation mechanism for the direct graphite-to-diamond phase transition. Nature Materials, 2011, 10, 693-697.	13.3	277
95	Ab initioquality neural-network potential for sodium. Physical Review B, 2010, 81, .	1.1	115
96	Graphite-diamond phase coexistence study employing a neural-network mapping of theab initiopotential energy surface. Physical Review B, 2010, 81, .	1.1	100
97	Signatures of nonadiabatic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>O</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:ma at Al(111): First-principles fewest-switches study. Physical Review B, 2010, 81, .	1.1	73
98	Pressureâ€induced phase transitions in silicon studied by neural networkâ€based metadynamics simulations. Physica Status Solidi (B): Basic Research, 2008, 245, 2618-2629.	0.7	68
99	Metadynamics Simulations of the High-Pressure Phases of Silicon Employing a High-Dimensional Neural Network Potential. Physical Review Letters, 2008, 100, 185501.	2.9	207
100	Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. Physical Review B, 2008, 77, .	1.1	112
101	Fingerprints for Spin-Selection Rules in the Interaction Dynamics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>at Al(111). Physical Review Letters, 2008, 101, 096104.	2.9	76
102	Nonadiabatic potential-energy surfaces by constrained density-functional theory. Physical Review B, 2007, 75, .	1.1	85
103	Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces. Physical Review Letters, 2007, 98, 146401.	2.9	2,677
104	Representing molecule-surface interactions with symmetry-adapted neural networks. Journal of Chemical Physics, 2007, 127, 014705.	1.2	128
105	Spectral broadening due to long-range Coulomb interactions in the molecular metal TTF-TCNQ. European Physical Journal B, 2007, 56, 173-176.	0.6	37
106	Behler, Reuter, and Scheffler Reply:. Physical Review Letters, 2006, 96, .	2.9	5
107	Structure determination of small vanadium clusters by density-functional theory in comparison with experimental far-infrared spectra. Journal of Chemical Physics, 2005, 122, 124302.	1.2	74
108	Dissociation ofO_2at Al(111): The Role of Spin Selection Rules. Physical Review Letters, 2005, 94, 036104.	2.9	259

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109	Structure Determination of Isolated Metal Clusters via Far-Infrared Spectroscopy. Physical Review Letters, 2004, 93, 023401.	2.9	161
110	Molecular Composition of Liquid Sulfur. Angewandte Chemie - International Edition, 2002, 41, 3199-3202.	7.2	26
111	Water structuring properties of carbohydrates, molecular dynamics studies on 1,5-anhydro-D-fructose. Physical Chemistry Chemical Physics, 2001, 3, 588-601.	1.3	20
112	Neural network potential-energy surfaces for atomistic simulations. Chemical Modelling, 0, , 1-41.	0.2	9