JÃ¶rg Behler

List of Publications by Year
in descending order

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112	14,701	26630	22832
papers	citations	56 h-index	112 g-index

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

#	Article	IF	Citations
1	Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces. Physical Review Letters, 2007, 98, 146401.	7.8	2,677
2	Atom-centered symmetry functions for constructing high-dimensional neural network potentials. Journal of Chemical Physics, 2011, 134, 074106.	3.0	1,014
3	Perspective: Machine learning potentials for atomistic simulations. Journal of Chemical Physics, 2016, 145, 170901.	3.0	879
4	Neural network potential-energy surfaces in chemistry: a tool for large-scale simulations. Physical Chemistry Chemical Physics, 2011, 13, 17930.	2.8	573
5	Constructing highâ€dimensional neural network potentials: A tutorial review. International Journal of Quantum Chemistry, 2015, 115, 1032-1050.	2.0	569
6	First Principles Neural Network Potentials for Reactive Simulations of Large Molecular and Condensed Systems. Angewandte Chemie - International Edition, 2017, 56, 12828-12840.	13.8	462
7	Performance and Cost Assessment of Machine Learning Interatomic Potentials. Journal of Physical Chemistry A, 2020, 124, 731-745.	2.5	428
8	Machine learning molecular dynamics for the simulation of infrared spectra. Chemical Science, 2017, 8, 6924-6935.	7.4	349
9	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.	7.1	312
10	Four Generations of High-Dimensional Neural Network Potentials. Chemical Reviews, 2021, 121, 10037-10072.	47.7	292
11	High-dimensional neural-network potentials for multicomponent systems: Applications to zinc oxide. Physical Review B, 2011, 83, .	3.2	286
12	Nucleation mechanism for the direct graphite-to-diamond phase transition. Nature Materials, 2011, 10, 693-697.	27.5	277
13	Dissociation ofO2at Al(111): The Role of Spin Selection Rules. Physical Review Letters, 2005, 94, 036104.	7.8	259
14	Representing potential energy surfaces by high-dimensional neural network potentials. Journal of Physics Condensed Matter, 2014, 26, 183001.	1.8	252
15	High-dimensional neural network potentials for metal surfaces: A prototype study for copper. Physical Review B, 2012, 85, .	3.2	249
16	Automatic selection of atomic fingerprints and reference configurations for machine-learning potentials. Journal of Chemical Physics, 2018, 148, 241730.	3.0	224
17	A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer. Nature Communications, 2021, 12, 398.	12.8	215
18	Metadynamics Simulations of the High-Pressure Phases of Silicon Employing a High-Dimensional Neural Network Potential. Physical Review Letters, 2008, 100, 185501.	7.8	207

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19	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.	7.1	201
20	Neural network interatomic potential for the phase change material GeTe. Physical Review B, 2012, 85, .	3.2	198
21	Library-Based LAMMPS Implementation of High-Dimensional Neural Network Potentials. Journal of Chemical Theory and Computation, 2019, 15, 1827-1840.	5.3	175
22	Structure Determination of Isolated Metal Clusters via Far-Infrared Spectroscopy. Physical Review Letters, 2004, 93, 023401.	7.8	161
23	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.	2.5	157
24	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.	3.0	142
25	Neural network molecular dynamics simulations of solidâ€“liquid interfaces: water at low-index copper surfaces. Physical Chemistry Chemical Physics, 2016, 18, 28704-28725.	2.8	141
26	Fast Crystallization of the Phase Change Compound GeTe by Large-Scale Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2013, 4, 4241-4246.	4.6	133
27	Representing molecule-surface interactions with symmetry-adapted neural networks. Journal of Chemical Physics, 2007, 127, 014705.	3.0	128
28	Accurate Neural Network Description of Surface Phonons in Reactive Gasâ€“Surface Dynamics: N₂ + Ru(0001). Journal of Physical Chemistry Letters, 2017, 8, 2131-2136.	4.6	126
29	Parallel Multistream Training of High-Dimensional Neural Network Potentials. Journal of Chemical Theory and Computation, 2019, 15, 3075-3092.	5.3	124
30	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.	3.0	117
31	Ab initioquality neural-network potential for sodium. Physical Review B, 2010, 81, .	3.2	115
32	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.	1.5	113
33	Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. Physical Review B, 2008, 77, .	3.2	112
34	Construction of high-dimensional neural network potentials using environment-dependent atom pairs. Journal of Chemical Physics, 2012, 136, 194111.	3.0	107
35	Proton-Transfer Mechanisms at the Waterâ€“ZnO Interface: The Role of Presolvation. Journal of Physical Chemistry Letters, 2017, 8, 1476-1483.	4.6	106
36	Graphite-diamond phase coexistence study employing a neural-network mapping of theab initiopotential energy surface. Physical Review B, 2010, 81, .	3.2	100

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37	Nonadiabatic potential-energy surfaces by constrained density-functional theory. Physical Review B, 2007, 75, .	3.2	85
38	Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. Physical Review B, 2015, 92, .	3.2	82
39	Machine learning potentials for extended systems: a perspective. European Physical Journal B, 2021, 94, 1.	1.5	81
40	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.	5.3	80
41	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.	7.8	76
42	Thermal transport in phase-change materials from atomistic simulations. Physical Review B, 2012, 86, .	3.2	75
43	Breakdown of Stokesâ€“Einstein relation in the supercooled liquid state of phase change materials. Physica Status Solidi (B): Basic Research, 2012, 249, 1880-1885.	1.5	75
44	Structure determination of small vanadium clusters by density-functional theory in comparison with experimental far-infrared spectra. Journal of Chemical Physics, 2005, 122, 124302.	3.0	74
45	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:math>at Al(111): First-principles fewest-switches study. Physical Review B, 2010, 81, .	3.2	73
46	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.	5.3	72
47	Representing the potential-energy surface of protonated water clusters by high-dimensional neural network potentials. Physical Chemistry Chemical Physics, 2015, 17, 8356-8371.	2.8	69
48	Neural Network Potentials: A Concise Overview of Methods. Annual Review of Physical Chemistry, 2022, 73, 163-186.	10.8	69
49	Pressureâ€induced phase transitions in silicon studied by neural networkâ€based metadynamics simulations. Physica Status Solidi (B): Basic Research, 2008, 245, 2618-2629.	1.5	68
50	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.	4.6	66
51	Next generation interatomic potentials for condensed systems. European Physical Journal B, 2014, 87, 1.	1.5	65
52	General-Purpose Machine Learning Potentials Capturing Nonlocal Charge Transfer. Accounts of Chemical Research, 2021, 54, 808-817.	15.6	65
53	Microscopic Origins of the Anomalous Melting Behavior of Sodium under High Pressure. Physical Review Letters, 2012, 108, 115701.	7.8	64
54	Structure of aqueous NaOH solutions: insights from neural-network-based molecular dynamics simulations. Physical Chemistry Chemical Physics, 2017, 19, 82-96.	2.8	64

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55	Structure and Dynamics of the Liquidâ€“Water/Zinc-Oxide Interface from Machine Learning Potential Simulations. Journal of Physical Chemistry C, 2019, 123, 1293-1304.	3.1	58
56	Dynamical Heterogeneity in the Supercooled Liquid State of the Phase Change Material GeTe. Journal of Physical Chemistry B, 2014, 118, 13621-13628.	2.6	57
57	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.	4.6	57
58	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.	4.6	56
59	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.	3.0	48
60	High order path integrals made easy. Journal of Chemical Physics, 2016, 145, 234103.	3.0	47
61	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.	4.6	45
62	Atomistic Simulations of the Crystallization and Aging of GeTe Nanowires. Journal of Physical Chemistry C, 2017, 121, 23827-23838.	3.1	42
63	Electron-phonon interaction and thermal boundary resistance at the crystal-amorphous interface of the phase change compound GeTe. Journal of Applied Physics, 2015, 117, .	2.5	41
64	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.	2.5	40
65	One-dimensional vs. two-dimensional proton transport processes at solidâ€“liquid zinc-oxideâ€“water interfaces. Chemical Science, 2019, 10, 1232-1243.	7.4	39
66	A critical comparison of neural network potentials for molecular reaction dynamics with exact permutation symmetry. Physical Chemistry Chemical Physics, 2019, 21, 9672-9682.	2.8	39
67	Spectral broadening due to long-range Coulomb interactions in the molecular metal TTF-TCNQ. European Physical Journal B, 2007, 56, 173-176.	1.5	37
68	An assessment of the structural resolution of various fingerprints commonly used in machine learning. Machine Learning: Science and Technology, 2021, 2, 015018.	5.0	37
69	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.	3.0	33
70	Insights into Water Permeation through hBN Nanocapillaries by Ab Initio Machine Learning Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2020, 11, 7363-7370.	4.6	33
71	Self-Diffusion of Surface Defects at Copperâ€“Water Interfaces. Journal of Physical Chemistry C, 2017, 121, 4368-4383.	3.1	31
72	High-dimensional neural network potentials for solvation: The case of protonated water clusters in helium. Journal of Chemical Physics, 2018, 148, 102310.	3.0	30

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73	High-dimensional neural network potentials for magnetic systems using spin-dependent atom-centered symmetry functions. Npj Computational Materials, 2021, 7, .	8.7	30
74	Nuclear Quantum Effects in Sodium Hydroxide Solutions from Neural Network Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 10158-10171.	2.6	29
75	Heterogeneous Crystallization of the Phase Change Material GeTe via Atomistic Simulations. Journal of Physical Chemistry C, 2015, 119, 6428-6434.	3.1	28
76	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.	3.0	28
77	Transferability of neural network potentials for varying stoichiometry: Phonons and thermal conductivity of MnxGey compounds. Journal of Applied Physics, 2020, 127, .	2.5	27
78	Properties of Î±-Brass Nanoparticles. 1. Neural Network Potential Energy Surface. Journal of Physical Chemistry C, 2020, 124, 12682-12695.	3.1	27
79	Molecular Composition of Liquid Sulfur. Angewandte Chemie - International Edition, 2002, 41, 3199-3202.	13.8	26
80	Predicting oxidation and spin states by high-dimensional neural networks: Applications to lithium manganese oxide spinels. Journal of Chemical Physics, 2020, 153, 164107.	3.0	26
81	A Full-Dimensional Neural Network Potential-Energy Surface for Water Clusters up to the Hexamer. Zeitschrift Fur Physikalische Chemie, 2013, 227, .	2.8	25
82	Temperature effects on the ionic conductivity in concentrated alkaline electrolyte solutions. Physical Chemistry Chemical Physics, 2020, 22, 10426-10430.	2.8	25
83	Closing the gap between theory and experiment for lithium manganese oxide spinels using a high-dimensional neural network potential. Physical Review B, 2020, 102, .	3.2	24
84	Temperature dependence of the vibrational spectrum of porphycene: a qualitative failure of classical-nuclei molecular dynamics. Faraday Discussions, 2020, 221, 526-546.	3.2	22
85	Mechanism of amorphous phase stabilization in ultrathin films of monoatomic phase change material. Nanoscale, 2021, 13, 16146-16155.	5.6	22
86	Mode specific dynamics in the H2 + SH â†' H + H2S reaction. Physical Chemistry Chemical Physics, 2016, 18, 29113-29121.	2.8	21
87	Water structuring properties of carbohydrates, molecular dynamics studies on 1,5-anhydro-D-fructose. Physical Chemistry Chemical Physics, 2001, 3, 588-601.	2.8	20
88	Atomistic simulations of thermal conductivity in GeTe nanowires. Journal Physics D: Applied Physics, 2020, 53, 054001.	2.8	20
89	Proton-Transfer-Driven Water Exchange Mechanism in the Na+ Solvation Shell. Journal of Physical Chemistry B, 2017, 121, 4184-4190.	2.6	18
90	Priming effects in the crystallization of the phase change compound GeTe from atomistic simulations. Faraday Discussions, 2019, 213, 287-301.	3.2	18

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91	Insights into lithium manganese oxideâ€“water interfaces using machine learning potentials. Journal of Chemical Physics, 2021, 155, 244703.	3.0	18
92	Hochdimensionale neuronale Netze fÃ¼r Potentialhyperflächen groÃŸer molekularer und kondensierter Systeme. Angewandte Chemie, 2017, 129, 13006-13020.	2.0	17
93	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.	3.1	15
94	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.	2.8	14
95	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.	2.8	13
96	Hybrid density functional theory benchmark study on lithium manganese oxides. Physical Review B, 2020, 101, .	3.2	12
97	Adsorption of Methanethiolate and Atomic Sulfur at the Cu(111) Surface: A Computational Study. Journal of Physical Chemistry C, 2013, 117, 337-348.	3.1	11
98	Peeling by Nanomechanical Forces: A Route to Selective Creation of Surface Structures. Physical Review Letters, 2015, 115, 036102.	7.8	10
99	Density anomaly of water at negative pressures from first principles. Journal of Physics Condensed Matter, 2018, 30, 254005.	1.8	10
100	Atomic mobility in the overheated amorphous GeTe compound for phase change memories. Physica Status Solidi (A) Applications and Materials Science, 2016, 213, 329-334.	1.8	9
101	Properties of Î±-Brass Nanoparticles II: Structure and Composition. Journal of Physical Chemistry C, 2021, 125, 14897-14909.	3.1	9
102	Neural network potential-energy surfaces for atomistic simulations. Chemical Modelling, 0, , 1-41.	0.4	9
103	Neural Network Potentials in Materials Modeling. , 2018, , 1-20.		7
104	A flexible and adaptive grid algorithm for global optimization utilizing basin hopping Monte Carlo. Journal of Chemical Physics, 2020, 152, 094109.	3.0	6
105	A Hessian-based assessment of atomic forces for training machine learning interatomic potentials. Journal of Chemical Physics, 2022, 156, 114106.	3.0	6
106	Behler, Reuter, and Scheffler Reply:. Physical Review Letters, 2006, 96, .	7.8	5
107	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.	2.8	4
108	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.	3.3	4

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109	Neural Network Potentials in Materials Modeling. , 2020, , 661-680.		4
110	High-Dimensional Neural Network Potentials for Atomistic Simulations. ACS Symposium Series, 2019, , 49-59.	0.5	2
111	A bin and hash method for analyzing reference data and descriptors in machine learning potentials. Machine Learning: Science and Technology, 2021, 2, 037001.	5.0	2
112	High-Dimensional Neural Network Potentials for Atomistic Simulations. Lecture Notes in Physics, 2020, , 253-275.	0.7	1