Jrg Behler

List of Publications by Year in Descending Order

112 papers	10,057 citations	49 h-index	100 g-index
119 ext. papers	12,130 ext. citations	5.6 avg, IF	7.54 L-index

#	Paper	IF	Citations
112	A Hessian-based assessment of atomic forces for training machine learning interatomic potentials.. *Journal of Chemical Physics*, **2022**, 156, 114106	3.9	
111	High-dimensional neural network potentials for magnetic systems using spin-dependent atom-centered symmetry functions. *Npj Computational Materials*, **2021**, 7,	10.9	3
110	An assessment of the structural resolution of various fingerprints commonly used in machine learning. *Machine Learning: Science and Technology*, **2021**, 2, 015018	5.1	24
109	Four Generations of High-Dimensional Neural Network Potentials. *Chemical Reviews*, **2021**, 121, 10037-10072	68.1	75
108	A bin and hash method for analyzing reference data and descriptors in machine learning potentials. *Machine Learning: Science and Technology*, **2021**, 2, 037001	5.1	0
107	Properties of □Brass Nanoparticles II: Structure and Composition. *Journal of Physical Chemistry C*, **2021**, 125, 14897-14909	3.8	1
106	Machine learning potentials for extended systems: a perspective. *European Physical Journal B*, **2021**, 94, 1	1.2	13
105	A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer. *Nature Communications*, **2021**, 12, 398	17.4	68
104	General-Purpose Machine Learning Potentials Capturing Nonlocal Charge Transfer. *Accounts of Chemical Research*, **2021**, 54, 808-817	24.3	24
103	Mechanism of amorphous phase stabilization in ultrathin films of monoatomic phase change material. *Nanoscale*, **2021**, 13, 16146-16155	7.7	5
102	Insights into lithium manganese oxide-water interfaces using machine learning potentials.. *Journal of Chemical Physics*, **2021**, 155, 244703	3.9	3
101	Hybrid density functional theory benchmark study on lithium manganese oxides. *Physical Review B*, **2020**, 101,	3.3	10
100	Accurate Global Potential Energy Surfaces for the H + CHOH Reaction by Neural Network Fitting with Permutation Invariance. *Journal of Physical Chemistry A*, **2020**, 124, 5737-5745	2.8	23
99	A flexible and adaptive grid algorithm for global optimization utilizing basin hopping Monte Carlo. *Journal of Chemical Physics*, **2020**, 152, 094109	3.9	3
98	Performance and Cost Assessment of Machine Learning Interatomic Potentials. *Journal of Physical Chemistry A*, **2020**, 124, 731-745	2.8	185
97	High-Dimensional Neural Network Potentials for Atomistic Simulations. *Lecture Notes in Physics*, **2020**, 253-275	0.8	0
96	Neural Network Potentials in Materials Modeling **2020**, 661-680		3

95	Temperature effects on the ionic conductivity in concentrated alkaline electrolyte solutions. *Physical Chemistry Chemical Physics*, **2020**, 22, 10426-10430	3.6	18
94	Atomistic simulations of thermal conductivity in GeTe nanowires. *Journal Physics D: Applied Physics*, **2020**, 53, 054001	3	12
93	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	6.4	44
92	Transferability of neural network potentials for varying stoichiometry: Phonons and thermal conductivity of MnxGey compounds. *Journal of Applied Physics*, **2020**, 127, 244901	2.5	12
91	Global optimization of copper clusters at the ZnO(101□0) surface using a DFT-based neural network potential and genetic algorithms. *Journal of Chemical Physics*, **2020**, 153, 054704	3.9	14
90	Insights into Water Permeation through hBN Nanocapillaries by Ab Initio Machine Learning Molecular Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2020**, 11, 7363-7370	6.4	17
89	Closing the gap between theory and experiment for lithium manganese oxide spinels using a high-dimensional neural network potential. *Physical Review B*, **2020**, 102,	3.3	10
88	Predicting oxidation and spin states by high-dimensional neural networks: Applications to lithium manganese oxide spinels. *Journal of Chemical Physics*, **2020**, 153, 164107	3.9	11
87	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	3.6	9
86	Properties of □Brass Nanoparticles. 1. Neural Network Potential Energy Surface. *Journal of Physical Chemistry C*, **2020**, 124, 12682-12695	3.8	14
85	Priming effects in the crystallization of the phase change compound GeTe from atomistic simulations. *Faraday Discussions*, **2019**, 213, 287-301	3.6	15
84	One-dimensional two-dimensional proton transport processes at solid-liquid zinc-oxide-water interfaces. *Chemical Science*, **2019**, 10, 1232-1243	9.4	29
83	Library-Based LAMMPS Implementation of High-Dimensional Neural Network Potentials. *Journal of Chemical Theory and Computation*, **2019**, 15, 1827-1840	6.4	94
82	A critical comparison of neural network potentials for molecular reaction dynamics with exact permutation symmetry. *Physical Chemistry Chemical Physics*, **2019**, 21, 9672-9682	3.6	30
81	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	6.4	40
80	Orbital-Dependent Electronic Friction Significantly Affects the Description of Reactive Scattering of N from Ru(0001). *Journal of Physical Chemistry Letters*, **2019**, 10, 2957-2962	6.4	33
79	Parallel Multistream Training of High-Dimensional Neural Network Potentials. *Journal of Chemical Theory and Computation*, **2019**, 15, 3075-3092	6.4	61
78	Accurate Probabilities for Highly Activated Reaction of Polyatomic Molecules on Surfaces Using a High-Dimensional Neural Network Potential: CHD + Cu(111). *Journal of Physical Chemistry Letters*, **2019**, 10, 1763-1768	6.4	42

77	New Insights into the Catalytic Activity of Cobalt Orthophosphate Co (PO) from Charge Density Analysis. *Chemistry - A European Journal*, **2019**, 25, 15786-15794	4.8	2
76	High-Dimensional Neural Network Potentials for Atomistic Simulations. *ACS Symposium Series*, **2019**, 49-59	0.4	1
75	Structure and Dynamics of the Liquid□Water/Zinc-Oxide Interface from Machine Learning Potential Simulations. *Journal of Physical Chemistry C*, **2019**, 123, 1293-1304	3.8	34
74	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	11.5	130
73	Temperature dependence of the vibrational spectrum of porphycene: a qualitative failure of classical-nuclei molecular dynamics. *Faraday Discussions*, **2019**, 221, 526-546	3.6	14
72	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	3.9	104
71	Maximally resolved anharmonic OH vibrational spectrum of the water/ZnO(101□0) interface from a high-dimensional neural network potential. *Journal of Chemical Physics*, **2018**, 148, 241720	3.9	20
70	High-dimensional neural network potentials for solvation: The case of protonated water clusters in helium. *Journal of Chemical Physics*, **2018**, 148, 102310	3.9	23
69	Analysis of Energy Dissipation Channels in a Benchmark System of Activated Dissociation: N on Ru(0001). *Journal of Physical Chemistry C*, **2018**, 122, 23470-23480	3.8	11
68	Nuclear Quantum Effects in Sodium Hydroxide Solutions from Neural Network Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 10158-10171	3.4	19
67	Neural Network Potentials in Materials Modeling **2018**, 1-20		7
66	Density anomaly of water at negative pressures from first principles. *Journal of Physics Condensed Matter*, **2018**, 30, 254005	1.8	7
65	Automatic selection of atomic fingerprints and reference configurations for machine-learning potentials. *Journal of Chemical Physics*, **2018**, 148, 241730	3.9	153
64	Self-Diffusion of Surface Defects at Copper□Water Interfaces. *Journal of Physical Chemistry C*, **2017**, 121, 4368-4383	3.8	27
63	Accurate Neural Network Description of Surface Phonons in Reactive Gas-Surface Dynamics: N + Ru(0001). *Journal of Physical Chemistry Letters*, **2017**, 8, 2131-2136	6.4	103
62	First Principles Neural Network Potentials for Reactive Simulations of Large Molecular and Condensed Systems. *Angewandte Chemie - International Edition*, **2017**, 56, 12828-12840	16.4	315
61	Hochdimensionale neuronale Netze f□ Potentialhyperfl□hen gro□r molekularer und kondensierter Systeme. *Angewandte Chemie*, **2017**, 129, 13006-13020	3.6	16
60	Proton-Transfer-Driven Water Exchange Mechanism in the Na Solvation Shell. *Journal of Physical Chemistry B*, **2017**, 121, 4184-4190	3.4	17

59	Proton-Transfer Mechanisms at the Water-ZnO Interface: The Role of Presolvation. *Journal of Physical Chemistry Letters*, **2017**, 8, 1476-1483	6.4	90
58	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	3.6	2
57	Atomistic Simulations of the Crystallization and Aging of GeTe Nanowires. *Journal of Physical Chemistry C*, **2017**, 121, 23827-23838	3.8	31
56	Machine learning molecular dynamics for the simulation of infrared spectra. *Chemical Science*, **2017**, 8, 6924-6935	9.4	237
55	Concentration-Dependent Proton Transfer Mechanisms in Aqueous NaOH Solutions: From Acceptor-Driven to Donor-Driven and Back. *Journal of Physical Chemistry Letters*, **2016**, 7, 3302-6	6.4	56
54	Structure of aqueous NaOH solutions: insights from neural-network-based molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2016**, 19, 82-96	3.6	48
53	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, 8368-73	11.5	230
52	Atomic mobility in the overheated amorphous GeTe compound for phase change memories. *Physica Status Solidi (A) Applications and Materials Science*, **2016**, 213, 329-334	1.6	8
51	High order path integrals made easy. *Journal of Chemical Physics*, **2016**, 145, 234103	3.9	37
50	Perspective: Machine learning potentials for atomistic simulations. *Journal of Chemical Physics*, **2016**, 145, 170901	3.9	591
49	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	3.9	39
48	Nuclear Quantum Effects in Water at the Triple Point: Using Theory as a Link Between Experiments. *Journal of Physical Chemistry Letters*, **2016**, 7, 2210-5	6.4	48
47	Neural network molecular dynamics simulations of solid-liquid interfaces: water at low-index copper surfaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 28704-28725	3.6	108
46	Mode specific dynamics in the H + SH -Ẇ + HS reaction. *Physical Chemistry Chemical Physics*, **2016**, 18, 29113-29121	3.6	17
45	Heterogeneous Crystallization of the Phase Change Material GeTe via Atomistic Simulations. *Journal of Physical Chemistry C*, **2015**, 119, 6428-6434	3.8	25
44	Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe. *Physical Review B*, **2015**, 92,	3.3	67
43	Representing the potential-energy surface of protonated water clusters by high-dimensional neural network potentials. *Physical Chemistry Chemical Physics*, **2015**, 17, 8356-71	3.6	60
42	Peeling by Nanomechanical Forces: A Route to Selective Creation of Surface Structures. *Physical Review Letters*, **2015**, 115, 036102	7.4	7

41	Constructing high-dimensional neural network potentials: A tutorial review. *International Journal of Quantum Chemistry*, **2015**, 115, 1032-1050	2.1	384
40	Electron-phonon interaction and thermal boundary resistance at the crystal-amorphous interface of the phase change compound GeTe. *Journal of Applied Physics*, **2015**, 117, 015304	2.5	38
39	Representing potential energy surfaces by high-dimensional neural network potentials. *Journal of Physics Condensed Matter*, **2014**, 26, 183001	1.8	185
38	Next generation interatomic potentials for condensed systems. *European Physical Journal B*, **2014**, 87, 1	1.2	55
37	Dynamical heterogeneity in the supercooled liquid state of the phase change material GeTe. *Journal of Physical Chemistry B*, **2014**, 118, 13621-8	3.4	49
36	Force-induced mechanical response of molecule-metal interfaces: molecular nanomechanics of propanethiolate self-assembled monolayers on Au(111). *Physical Chemistry Chemical Physics*, **2013**, 15, 16001-11	3.6	8
35	A Full-Dimensional Neural Network Potential-Energy Surface for Water Clusters up to the Hexamer. *Zeitschrift Fur Physikalische Chemie*, **2013**, 227,	3.1	24
34	Fast Crystallization of the Phase Change Compound GeTe by Large-Scale Molecular Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2013**, 4, 4241-6	6.4	114
33	Adsorption of Methanethiolate and Atomic Sulfur at the Cu(111) Surface: A Computational Study. *Journal of Physical Chemistry C*, **2013**, 117, 337-348	3.8	10
32	A density-functional theory-based neural network potential for water clusters including van der Waals corrections. *Journal of Physical Chemistry A*, **2013**, 117, 7356-66	2.8	128
31	Neural network potentials for metals and oxides – First applications to copper clusters at zinc oxide. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 1191-1203	1.3	93
30	Construction of high-dimensional neural network potentials using environment-dependent atom pairs. *Journal of Chemical Physics*, **2012**, 136, 194111	3.9	91
29	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	3.9	95
28	Thermal transport in phase-change materials from atomistic simulations. *Physical Review B*, **2012**, 86,	3.3	57
27	Neural network interatomic potential for the phase change material GeTe. *Physical Review B*, **2012**, 85,	3.3	149
26	High-dimensional neural network potentials for metal surfaces: A prototype study for copper. *Physical Review B*, **2012**, 85,	3.3	177
25	Breakdown of Stokes–Einstein relation in the supercooled liquid state of phase change materials. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 1880-1885	1.3	66
24	Microscopic origins of the anomalous melting behavior of sodium under high pressure. *Physical Review Letters*, **2012**, 108, 115701	7.4	53

23	Neural network potential-energy surfaces in chemistry: a tool for large-scale simulations. *Physical Chemistry Chemical Physics*, **2011**, 13, 17930-55	3.6	456
22	Atom-centered symmetry functions for constructing high-dimensional neural network potentials. *Journal of Chemical Physics*, **2011**, 134, 074106	3.9	657
21	High-dimensional neural-network potentials for multicomponent systems: Applications to zinc oxide. *Physical Review B*, **2011**, 83,	3.3	219
20	Nucleation mechanism for the direct graphite-to-diamond phase transition. *Nature Materials*, **2011**, 10, 693-7	27	235
19	Ab initio quality neural-network potential for sodium. *Physical Review B*, **2010**, 81,	3.3	103
18	Graphite-diamond phase coexistence study employing a neural-network mapping of the ab initio potential energy surface. *Physical Review B*, **2010**, 81,	3.3	89
17	Signatures of nonadiabatic O2 dissociation at Al(111): First-principles fewest-switches study. *Physical Review B*, **2010**, 81,	3.3	69
16	Metadynamics simulations of the high-pressure phases of silicon employing a high-dimensional neural network potential. *Physical Review Letters*, **2008**, 100, 185501	7.4	181
15	Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. *Physical Review B*, **2008**, 77,	3.3	103
14	Fingerprints for spin-selection rules in the interaction dynamics of O2 at Al(111). *Physical Review Letters*, **2008**, 101, 096104	7.4	68
13	Pressure-induced phase transitions in silicon studied by neural network-based metadynamics simulations. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 2618-2629	1.3	59
12	Representing molecule-surface interactions with symmetry-adapted neural networks. *Journal of Chemical Physics*, **2007**, 127, 014705	3.9	117
11	Spectral broadening due to long-range Coulomb interactions in the molecular metal TTF-TCNQ. *European Physical Journal B*, **2007**, 56, 173-176	1.2	36
10	Nonadiabatic potential-energy surfaces by constrained density-functional theory. *Physical Review B*, **2007**, 75,	3.3	75
9	Generalized neural-network representation of high-dimensional potential-energy surfaces. *Physical Review Letters*, **2007**, 98, 146401	7.4	1638
8	Behler, Reuter, and Scheffler Reply:. *Physical Review Letters*, **2006**, 96,	7.4	5
7	Dissociation of O2 at Al(111): the role of spin selection rules. *Physical Review Letters*, **2005**, 94, 036104	7.4	234
6	Structure determination of small vanadium clusters by density-functional theory in comparison with experimental far-infrared spectra. *Journal of Chemical Physics*, **2005**, 122, 124302	3.9	69

5	Structure determination of isolated metal clusters via far-infrared spectroscopy. *Physical Review Letters*, **2004**, 93, 023401	7.4	148
4	Molecular composition of liquid sulfur. *Angewandte Chemie - International Edition*, **2002**, 41, 3199-202	16.4	21
3	Water structuring properties of carbohydrates, molecular dynamics studies on 1,5-anhydro-D-fructose. *Physical Chemistry Chemical Physics*, **2001**, 3, 588-601	3.6	18
2	Neural network potential-energy surfaces for atomistic simulations. *Chemical Modelling*,1-41	2	9
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