Alexander Shapeev

List of Publications by Year
in descending order

64	4,573	159585 30	114465 63
papers	citations	h-index	g-index

64	64	64	2719
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exploring thermal expansion of carbon-based nanosheets by machine-learning interatomic potentials. Carbon, 2022, 186, 501-508.	10.3	30
2	Validation of moment tensor potentials for fcc and bcc metals using EXAFS spectra. Computational Materials Science, 2022, 210, 111028.	3.0	5
3	A machine-learning-based investigation on the mechanical/failure response and thermal conductivity of semiconducting BC2N monolayers. Carbon, 2022, 188, 431-441.	10.3	34
4	Nanohardness from First Principles with Active Learning on Atomic Environments. Journal of Chemical Theory and Computation, 2022, 18, 1109-1121.	5.3	10
5	Magnetic Moment Tensor Potentials for collinear spin-polarized materials reproduce different magnetic states of bcc Fe. Npj Computational Materials, 2022, 8, .	8.7	52
6	A first-principles and machine-learning investigation on the electronic, photocatalytic, mechanical and heat conduction properties of nanoporous C₅N monolayers. Nanoscale, 2022, 14, 4324-4333.	5.6	26
7	Anisotropic mechanical response, high negative thermal expansion, and outstanding dynamical stability of biphenylene monolayer revealed by machine-learning interatomic potentials. FlatChem, 2022, 32, 100347.	5.6	24
8	Outstanding thermal conductivity and mechanical properties in the direct gap semiconducting penta-NiN2 monolayer confirmed by first-principles. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 140, 115221.	2.7	10
9	A combined first-principles and machine-learning investigation on the stability, electronic, optical, and mechanical properties of novel C6N7-based nanoporous carbon nitrides. Carbon, 2022, 194, 230-239.	10.3	24
10	Mechanical, optical, and thermoelectric properties of semiconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>ZnIn</mml:mi><mml:mn>2</mml:mn></mml:mm <mml:math		

#	Article	IF	Citations
19	Firstâ€Principles Multiscale Modeling of Mechanical Properties in Graphene/Borophene Heterostructures Empowered by Machineâ€Learning Interatomic Potentials. Advanced Materials, 2021, 33, e2102807.	21.0	171
20	Bayesian learning of thermodynamic integration and numerical convergence for accurate phase diagrams. Physical Review B, 2021, 104, .	3.2	6
21	Efficient prediction of elastic properties of Ti0.5Al0.5N at elevated temperature using machine learning interatomic potential. Thin Solid Films, 2021, 737, 138927.	1.8	4
22	The MLIP package: moment tensor potentials with MPI and active learning. Machine Learning: Science and Technology, 2021, 2, 025002.	5.0	181
23	Machine-learned interatomic potentials for alloys and alloy phase diagrams. Npj Computational Materials, 2021, 7, .	8.7	75
24	Machine-learning potentials enable predictive and tractable high-throughput screening of random alloys. Physical Review Materials, 2021, 5, .	2.4	8
25	Mechanical, thermal transport, electronic and photocatalytic properties of penta-PdPS, -PdPSe and -PdPTe monolayers explored by first-principles calculations. Journal of Materials Chemistry C, 2021, 10, 329-336.	5.5	14
26	Metallization of diamond. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 24634-24639.	7.1	29
27	Lattice dynamics of YbxCo4Sb12 skutterudite by machine-learning interatomic potentials: Effect of filler concentration and disorder. Physical Review B, 2020, 102, .	3.2	15
28	Exploring phononic properties of two-dimensional materials using machine learning interatomic potentials. Applied Materials Today, 2020, 20, 100685.	4.3	96
29	Ab initio analysis of structural and electronic properties and excitonic optical responses of eight Ge-based 2D materials. Journal of Applied Physics, 2020, 127, 214301.	2.5	8
30	Nanoporous C3N4, C3N5 and C3N6 nanosheets; novel strong semiconductors with low thermal conductivities and appealing optical/electronic properties. Carbon, 2020, 167, 40-50.	10.3	72
31	High thermal conductivity in semiconducting Janus and non-Janus diamanes. Carbon, 2020, 167, 51-61.	10.3	39
32	Machine-learning interatomic potentials enable first-principles multiscale modeling of lattice thermal conductivity in graphene/borophene heterostructures. Materials Horizons, 2020, 7, 2359-2367.	12.2	124
33	Efficient machine-learning based interatomic potentialsfor exploring thermal conductivity in two-dimensional materials. JPhys Materials, 2020, 3, 02LT02.	4.2	32
34	Youngâ€™s Modulus and Tensile Strength of Ti₃C₂ MXene Nanosheets As Revealed by In Situ TEM Probing, AFM Nanomechanical Mapping, and Theoretical Calculations. Nano Letters, 2020, 20, 5900-5908.	9.1	88
35	Performance and Cost Assessment of Machine Learning Interatomic Potentials. Journal of Physical Chemistry A, 2020, 124, 731-745.	2.5	428
36	Predicting the propensity for thermally activated Î² events in metallic glasses via interpretable machine learning. Npj Computational Materials, 2020, 6, .	8.7	35

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37	Elinvar effect in Î²-Ti simulated by on-the-fly trained moment tensor potential. New Journal of Physics, 2020, 22, 113005.	2.9	20
38	In operando active learning of interatomic interaction during large-scale simulations. Machine Learning: Science and Technology, 2020, 1, 045005.	5.0	11
39	Short-range order in face-centered cubic VCoNi alloys. Physical Review Materials, 2020, 4, .	2.4	24
40	Prediction of C₇N₆ and C₉N₄: stable and strong porous carbon-nitride nanosheets with attractive electronic and optical properties. Journal of Materials Chemistry C, 2019, 7, 10908-10917.	5.5	57
41	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. Npj Computational Materials, 2019, 5, .	8.7	79
42	Accessing thermal conductivity of complex compounds by machine learning interatomic potentials. Physical Review B, 2019, 100, .	3.2	73
43	Impact of lattice relaxations on phase transitions in a high-entropy alloy studied by machine-learning potentials. Npj Computational Materials, 2019, 5, .	8.7	110
44	Applying a machine learning interatomic potential to unravel theÂeffects of local lattice distortion on the elastic properties of multi-principal element alloys. Journal of Alloys and Compounds, 2019, 803, 1054-1062.	5.5	41
45	Machine-learned multi-system surrogate models for materials prediction. Npj Computational Materials, 2019, 5, .	8.7	96
46	Accelerating crystal structure prediction by machine-learning interatomic potentials with active learning. Physical Review B, 2019, 99, .	3.2	229
47	Deep elastic strain engineering of bandgap through machine learning. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4117-4122.	7.1	70
48	Ring polymer molecular dynamics and active learning of moment tensor potential for gas-phase barrierless reactions: Application to S + H2. Journal of Chemical Physics, 2019, 151, 224105.	3.0	14
49	Improving accuracy of interatomic potentials: more physics or more data? A case study of silica. Materials Today Communications, 2019, 18, 74-80.	1.9	32
50	Accelerating high-throughput searches for new alloys with active learning of interatomic potentials. Computational Materials Science, 2019, 156, 148-156.	3.0	218
51	Machine learning of molecular properties: Locality and active learning. Journal of Chemical Physics, 2018, 148, 241727.	3.0	116
52	Active learning of linearly parametrized interatomic potentials. Computational Materials Science, 2017, 140, 171-180.	3.0	360
53	Accurate representation of formation energies of crystalline alloys with many components. Computational Materials Science, 2017, 139, 26-30.	3.0	40
54	Approximation of Crystalline Defects at Finite Temperature. Multiscale Modeling and Simulation, 2017, 15, 1830-1864.	1.6	3

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55	Moment Tensor Potentials: A Class of Systematically Improvable Interatomic Potentials. Multiscale Modeling and Simulation, 2016, 14, 1153-1173.	1.6	705
56	An Optimization Based Coupling Method for Multiscale Problems. Multiscale Modeling and Simulation, 2016, 14, 1377-1416.	1.6	3
57	An Optimization-based Atomistic-to-Continuum Coupling Method. SIAM Journal on Numerical Analysis, 2014, 52, 2183-2204.	2.3	20
58	(In-)stability and Stabilization of QNL-Type Atomistic-to-Continuum Coupling Methods. Multiscale Modeling and Simulation, 2014, 12, 1258-1293.	1.6	5
59	Theory-based benchmarking of the blended force-based quasicontinuum method. Computer Methods in Applied Mechanics and Engineering, 2014, 268, 763-781.	6.6	22
60	A Priori and A Posteriori $W^{1,infty}$ Error Analysis of a QC Method for Complex Lattices. SIAM Journal on Numerical Analysis, 2013, 51, 2357-2379.	2.3	5
61	Numerical Methods for Multilattices. Multiscale Modeling and Simulation, 2012, 10, 696-726.	1.6	10
62	Consistent Energy-Based Atomistic/Continuum Coupling for Two-Body Potentials in Three Dimensions. SIAM Journal of Scientific Computing, 2012, 34, B335-B360.	2.8	19
63	Consistent Energy-Based Atomistic/Continuum Coupling for Two-Body Potentials in One and Two Dimensions. Multiscale Modeling and Simulation, 2011, 9, 905-932.	1.6	57
64	An Asymptotic Fitting Finite Element Method with Exponential Mesh Refinement for Accurate Computation of Corner Eddies in Viscous Flows. SIAM Journal of Scientific Computing, 2009, 31, 1874-1900.	2.8	20