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	Moment Tensor Potentials: A Class of Systematically Improvable Interatomic Potentials. Multiscale Modeling and Simulation, 2016, 14, 1153-1173.	1.6	705
2	Performance and Cost Assessment of Machine Learning Interatomic Potentials. Journal of Physical Chemistry A, 2020, 124, 731-745.	2.5	428
3	Active learning of linearly parametrized interatomic potentials. Computational Materials Science, 2017, 140, 171-180.	3.0	360
4	Exceptional piezoelectricity, high thermal conductivity and stiffness and promising photocatalysis in two-dimensional MoSi2N4 family confirmed by first-principles. Nano Energy, 2021, 82, 105716.	16.0	303
5	Accelerating crystal structure prediction by machine-learning interatomic potentials with active learning. Physical Review B, 2019, 99, .	3.2	229
6	Accelerating high-throughput searches for new alloys with active learning of interatomic potentials. Computational Materials Science, 2019, 156, 148-156.	3.0	218
7	The MLIP package: moment tensor potentials with MPI and active learning. Machine Learning: Science and Technology, 2021, 2, 025002.	5.0	181
8	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
9	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
10	Machine learning of molecular properties: Locality and active learning. Journal of Chemical Physics, 2018, 148, 241727.	3.0	116
11	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
12	Accelerating first-principles estimation of thermal conductivity by machine-learning interatomic potentials: A MTP/ShengBTE solution. Computer Physics Communications, 2021, 258, 107583.	7.5	108
13	Machine-learned multi-system surrogate models for materials prediction. Npj Computational Materials, 2019, 5, .	8.7	96
14	Exploring phononic properties of two-dimensional materials using machine learning interatomic potentials. Applied Materials Today, 2020, 20, 100685.	4.3	96
15	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
16	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. Npj Computational Materials, 2019, 5, .	8.7	79
17	Machine-learned interatomic potentials for alloys and alloy phase diagrams. Npj Computational Materials, 2021, 7, .	8.7	75
18	Accessing thermal conductivity of complex compounds by machine learning interatomic potentials. Physical Review B, 2019, 100, .	3.2	73

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	Magnetic Moment Tensor Potentials for collinear spin-polarized materials reproduce different magnetic states of bcc Fe. Npj Computational Materials, 2022, 8, .	8.7	52
24	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
25	Accurate representation of formation energies of crystalline alloys with many components. Computational Materials Science, 2017, 139, 26-30.	3.0	40
26	High thermal conductivity in semiconducting Janus and non-Janus diamanes. Carbon, 2020, 167, 51-61.	10.3	39
27	Predicting the propensity for thermally activated Î² events in metallic glasses via interpretable machine learning. Npj Computational Materials, 2020, 6, .	8.7	35
28	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
29	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
30	Efficient machine-learning based interatomic potentialsfor exploring thermal conductivity in two-dimensional materials. JPhys Materials, 2020, 3, 02LT02.	4.2	32
31	Exploring thermal expansion of carbon-based nanosheets by machine-learning interatomic potentials. Carbon, 2022, 186, 501-508.	10.3	30
32	Metallization of diamond. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 24634-24639.	7.1	29
33	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
34	Short-range order in face-centered cubic VCoNi alloys. Physical Review Materials, 2020, 4, .	2.4	24
35	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
36	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

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37	Theory-based benchmarking of the blended force-based quasicontinuum method. Computer Methods in Applied Mechanics and Engineering, 2014, 268, 763-781.	6.6	22
38	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></mm <mml:math		

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55	Bayesian learning of thermodynamic integration and numerical convergence for accurate phase diagrams. Physical Review B, 2021, 104, .	3.2	6
56	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
57	(In-)stability and Stabilization of QNL-Type Atomistic-to-Continuum Coupling Methods. Multiscale Modeling and Simulation, 2014, 12, 1258-1293.	1.6	5
58	Free energy of (CoxMn1âˆ’x)3O4 mixed phases from machine-learning-enhanced ab initio calculations. Physical Review Materials, 2021, 5, .	2.4	5
59	Validation of moment tensor potentials for fcc and bcc metals using EXAFS spectra. Computational Materials Science, 2022, 210, 111028.	3.0	5
60	Modeling the high-temperature phase coexistence region of mixed transition metal oxides fromab initiocalculations. Physical Review Research, 2021, 3, .	3.6	4
61	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
62	An Optimization Based Coupling Method for Multiscale Problems. Multiscale Modeling and Simulation, 2016, 14, 1377-1416.	1.6	3
63	Approximation of Crystalline Defects at Finite Temperature. Multiscale Modeling and Simulation, 2017, 15, 1830-1864.	1.6	3
64	Assessing parameters for ring polymer molecular dynamics simulations at low temperatures: DHÂ+ÂH chemical reaction. Chemical Physics Letters, 2021, 773, 138567.	2.6	0