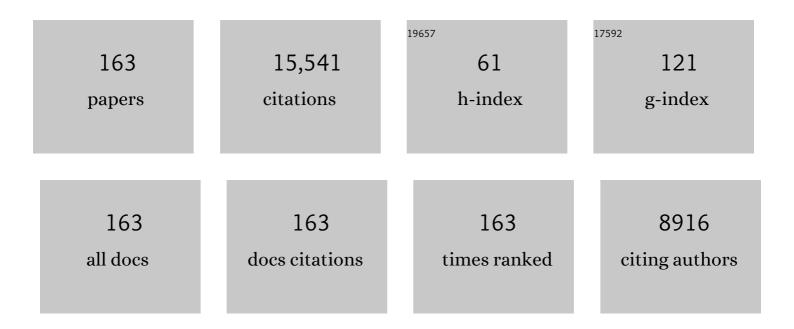
List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics. Physical Review Letters, 2018, 120, 143001.	7.8	1,006
2	String method for the study of rare events. Physical Review B, 2002, 66, .	3.2	843
3	The Heterognous Multiscale Methods. Communications in Mathematical Sciences, 2003, 1, 87-132.	1.0	826
4	Solving high-dimensional partial differential equations using deep learning. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 8505-8510.	7.1	807
5	DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics. Computer Physics Communications, 2018, 228, 178-184.	7.5	727
6	Simplified and improved string method for computing the minimum energy paths in barrier-crossing events. Journal of Chemical Physics, 2007, 126, 164103.	3.0	516
7	Transition-Path Theory and Path-Finding Algorithms for the Study of Rare Events. Annual Review of Physical Chemistry, 2010, 61, 391-420.	10.8	481
8	Deep Learning-Based Numerical Methods for High-Dimensional Parabolic Partial Differential Equations and Backward Stochastic Differential Equations. Communications in Mathematics and Statistics, 2017, 5, 349-380.	1.5	402
9	Finite Temperature String Method for the Study of Rare Eventsâ€. Journal of Physical Chemistry B, 2005, 109, 6688-6693.	2.6	397
10	Towards a Theory of Transition Paths. Journal of Statistical Physics, 2006, 123, 503-523.	1.2	375
11	The heterogeneous multiscale method. Acta Numerica, 2012, 21, 1-87.	10.7	334
12	Active learning of uniformly accurate interatomic potentials for materials simulation. Physical Review Materials, 2019, 3, .	2.4	299
13	DP-GEN: A concurrent learning platform for the generation of reliable deep learning based potential energy models. Computer Physics Communications, 2020, 253, 107206.	7.5	271
14	A Proposal on Machine Learning via Dynamical Systems. Communications in Mathematics and Statistics, 2017, 5, 1-11.	1.5	260
15	Invariant Measures for Burgers Equation with Stochastic Forcing. Annals of Mathematics, 2000, 151, 877.	4.2	236
16	Analysis of the heterogeneous multiscale method for elliptic homogenization problems. Journal of the American Mathematical Society, 2004, 18, 121-156.	3.9	196
17	Transition pathways in complex systems: Reaction coordinates, isocommittor surfaces, and transition tubes. Chemical Physics Letters, 2005, 413, 242-247.	2.6	187
18	Boundary conditions for the moving contact line problem. Physics of Fluids, 2007, 19, 022101.	4.0	186

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19	Minimum action method for the study of rare events. Communications on Pure and Applied Mathematics, 2004, 57, 637-656.	3.1	185
20	Heterogeneous multiscale method: A general methodology for multiscale modeling. Physical Review B, 2003, 67, .	3.2	182
21	Gibbsian Dynamics and Ergodicity¶for the Stochastically Forced Navier–Stokes Equation. Communications in Mathematical Physics, 2001, 224, 83-106.	2.2	174
22	Vorticity Boundary Condition and Related Issues for Finite Difference Schemes. Journal of Computational Physics, 1996, 124, 368-382.	3.8	170
23	Transition pathways in complex systems: Application of the finite-temperature string method to the alanine dipeptide. Journal of Chemical Physics, 2005, 123, 134109.	3.0	168
24	Deep Potential: A General Representation of a Many-Body Potential Energy Surface. Communications in Computational Physics, 2018, 23, .	1.7	164
25	Cauchy–Born Rule and the Stability of Crystalline Solids: Static Problems. Archive for Rational Mechanics and Analysis, 2007, 183, 241-297.	2.4	163
26	Adaptive local basis set for Kohn–Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation. Journal of Computational Physics, 2012, 231, 2140-2154.	3.8	162
27	Machine Learning Approximation Algorithms for High-Dimensional Fully Nonlinear Partial Differential Equations and Second-order Backward Stochastic Differential Equations. Journal of Nonlinear Science, 2019, 29, 1563-1619.	2.1	160
28	Heterogeneous multiscale method for the modeling of complex fluids and micro-fluidics. Journal of Computational Physics, 2005, 204, 1-26.	3.8	157
29	DeePCG: Constructing coarse-grained models via deep neural networks. Journal of Chemical Physics, 2018, 149, 034101.	3.0	141
30	Phase Diagram of a Deep Potential Water Model. Physical Review Letters, 2021, 126, 236001.	7.8	140
31	Nested stochastic simulation algorithm for chemical kinetic systems with disparate rates. Journal of Chemical Physics, 2005, 123, 194107.	3.0	135
32	A Gauss–Seidel Projection Method for Micromagnetics Simulations. Journal of Computational Physics, 2001, 171, 357-372.	3.8	131
33	Matching Conditions in Atomistic-Continuum Modeling of Materials. Physical Review Letters, 2001, 87, 135501.	7.8	125
34	Probability Distribution Functions for the Random Forced Burgers Equation. Physical Review Letters, 1997, 78, 1904-1907.	7.8	120
35	Essentially Compact Schemes for Unsteady Viscous Incompressible Flows. Journal of Computational Physics, 1996, 126, 122-138.	3.8	113
36	Microscopic mechanisms of equilibrium melting of a solid. Science, 2014, 346, 729-732.	12.6	111

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37	Solving many-electron Schrödinger equation using deep neural networks. Journal of Computational Physics, 2019, 399, 108929.	3.8	108
38	Nucleation of Ordered Phases in Block Copolymers. Physical Review Letters, 2010, 104, 148301.	7.8	106
39	Multiscale simulations in simple metals: A density-functional-based methodology. Physical Review B, 2005, 71, .	3.2	103
40	A Dynamic Atomistic–Continuum Method for the Simulation of Crystalline Materials. Journal of Computational Physics, 2002, 182, 234-261.	3.8	102
41	Nested stochastic simulation algorithms for chemical kinetic systems with multiple time scales. Journal of Computational Physics, 2007, 221, 158-180.	3.8	101
42	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. Computer Physics Communications, 2021, 259, 107624.	7.5	100
43	Finite difference heterogeneous multi-scale method for homogenization problems. Journal of Computational Physics, 2003, 191, 18-39.	3.8	98
44	Multiscale modeling of the dynamics of solids at finite temperature. Journal of the Mechanics and Physics of Solids, 2005, 53, 1650-1685.	4.8	96
45	Optimal partition and effective dynamics of complex networks. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 7907-7912.	7.1	91
46	Self-induced stochastic resonance in excitable systems. Physica D: Nonlinear Phenomena, 2005, 210, 227-240.	2.8	90
47	Gauge Method for Viscous Incompressible Flows. Communications in Mathematical Sciences, 2003, 1, 317-332.	1.0	90
48	DeFine: deep convolutional neural networks accurately quantify intensities of transcription factor-DNA binding and facilitate evaluation of functional non-coding variants. Nucleic Acids Research, 2018, 46, e69-e69.	14.5	89
49	Continuum models for the contact line problem. Physics of Fluids, 2010, 22, .	4.0	87
50	Uniform accuracy of the quasicontinuum method. Physical Review B, 2006, 74, .	3.2	86
51	Ergodicity for the Navier-Stokes equation with degenerate random forcing: Finite-dimensional approximation. Communications on Pure and Applied Mathematics, 2001, 54, 1386-1402.	3.1	85
52	Adaptive minimum action method for the study of rare events. Journal of Chemical Physics, 2008, 128, 104111.	3.0	84
53	Energy landscape and thermally activated switching of submicron-sized ferromagnetic elements. Journal of Applied Physics, 2003, 93, 2275-2282.	2.5	83
54	The local microscale problem in the multiscale modeling of strongly heterogeneous media: Effects of boundary conditions and cell size. Journal of Computational Physics, 2007, 222, 556-572.	3.8	82

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55	Well-Posedness for the Dumbbell Model of Polymeric Fluids. Communications in Mathematical Physics, 2004, 248, 409-427.	2.2	81
56	A general strategy for designing seamless multiscale methods. Journal of Computational Physics, 2009, 228, 5437-5453.	3.8	80
57	Analysis of the heterogeneous multiscale method for ordinary differential equations. Communications in Mathematical Sciences, 2003, 1, 423-436.	1.0	74
58	Kinetic model for a step edge in epitaxial growth. Physical Review E, 1999, 59, 6879-6887.	2.1	69
59	Modeling subgrid-scale forces by spatial artificial neural networks in large eddy simulation of turbulence. Physical Review Fluids, 2020, 5, .	2.5	68
60	On Multilevel Picard Numerical Approximations for High-Dimensional Nonlinear Parabolic Partial Differential Equations and High-Dimensional Nonlinear Backward Stochastic Differential Equations. Journal of Scientific Computing, 2019, 79, 1534-1571.	2.3	66
61	Generalized flows, intrinsic stochasticity, and turbulent transport. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 8200-8205.	7.1	62
62	Asymptotic Theory for the Probability Density Functions in Burgers Turbulence. Physical Review Letters, 1999, 83, 2572-2575.	7.8	61
63	Deep potentials for materials science. Materials Futures, 2022, 1, 022601.	8.4	61
64	Deep neural network for the dielectric response of insulators. Physical Review B, 2020, 102, .	3.2	60
65	Coupling kinetic Monte-Carlo and continuum models with application to epitaxial growth. Journal of Computational Physics, 2003, 189, 197-211.	3.8	59
66	Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems. Communications in Mathematical Sciences, 2009, 7, 755-777.	1.0	59
67	On the Crystallization of 2D Hexagonal Lattices. Communications in Mathematical Physics, 2009, 286, 1099-1140.	2.2	57
68	A deep potential model with long-range electrostatic interactions. Journal of Chemical Physics, 2022, 156, 124107.	3.0	57
69	Dynamics of vortex liquids in Ginzburg-Landau theories with applications to superconductivity. Physical Review B, 1994, 50, 1126-1135.	3.2	53
70	Localized bases of eigensubspaces and operator compression. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1273-1278.	7.1	52
71	Isotope effects in liquid water via deep potential molecular dynamics. Molecular Physics, 2019, 117, 3269-3281.	1.7	52
72	Uniformly accurate machine learning-based hydrodynamic models for kinetic equations. Proceedings of the United States of America, 2019, 116, 21983-21991.	7.1	51

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73	Deep potential generation scheme and simulation protocol for the Li10GeP2S12-type superionic conductors. Journal of Chemical Physics, 2021, 154, 094703.	3.0	49
74	Reinforced dynamics for enhanced sampling in large atomic and molecular systems. Journal of Chemical Physics, 2018, 148, 124113.	3.0	48
75	Pole-Based approximation of the Fermi-Dirac function. Chinese Annals of Mathematics Series B, 2009, 30, 729-742.	0.4	46
76	Nonlinear evolution equation for the stress-driven morphological instability. Journal of Applied Physics, 2002, 91, 9414-9422.	2.5	45
77	Variational boundary conditions for molecular dynamics simulations of crystalline solids at finite temperature: Treatment of the thermal bath. Physical Review B, 2007, 76, .	3.2	44
78	Ground State Energy Functional with Hartree–Fock Efficiency and Chemical Accuracy. Journal of Physical Chemistry A, 2020, 124, 7155-7165.	2.5	42
79	Exponential convergence of the deep neural network approximation for analytic functions. Science China Mathematics, 2018, 61, 1733-1740.	1.7	41
80	Finite Difference Methods for 3D Viscous Incompressible Flows in the Vorticity–Vector Potential Formulation on Nonstaggered Grids. Journal of Computational Physics, 1997, 138, 57-82.	3.8	40
81	Brownian motors in the photoalignment of liquid crystals. Applied Physics A: Materials Science and Processing, 2002, 75, 293-300.	2.3	40
82	DeePKS: A Comprehensive Data-Driven Approach toward Chemically Accurate Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 170-181.	5.3	40
83	<i>A priori</i> estimates of the population risk for two-layer neural networks. Communications in Mathematical Sciences, 2019, 17, 1407-1425.	1.0	40
84	Model Reduction with Memory and the Machine Learning of Dynamical Systems. Communications in Computational Physics, 2019, 25, .	1.7	39
85	Effective dynamics for ferromagnetic thin films. Journal of Applied Physics, 2001, 90, 370-374.	2.5	37
86	Algorithms for solving high dimensional PDEs: from nonlinear Monte Carlo to machine learning. Nonlinearity, 2022, 35, 278-310.	1.4	37
87	Modified models of polymer phase separation. Physical Review E, 2006, 73, 061801.	2.1	36
88	A Fast Parallel Algorithm for Selected Inversion of Structured Sparse Matrices with Application to 2D Electronic Structure Calculations. SIAM Journal of Scientific Computing, 2011, 33, 1329-1351.	2.8	35
89	Thermodynamically driven incompressible fluid mixtures. Journal of Chemical Physics, 1997, 107, 10177-10184.	3.0	33
90	Noise can play an organizing role for the recurrent dynamics in excitable media. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 702-707.	7.1	33

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91	Contact line dynamics on heterogeneous surfaces. Physics of Fluids, 2011, 23, .	4.0	33
92	Noisy Hegselmann-Krause Systems: Phase Transition and the 2R-Conjecture. Journal of Statistical Physics, 2017, 166, 1209-1225.	1.2	33
93	Finite Difference Schemes for Incompressible Flows in the Velocity–Impulse Density Formulation. Journal of Computational Physics, 1997, 130, 67-76.	3.8	32
94	Linear-scaling subspace-iteration algorithm with optimally localized nonorthogonal wave functions for Kohn-Sham density functional theory. Physical Review B, 2009, 79, .	3.2	32
95	Atomistic simulations of rare events using gentlest ascent dynamics. Journal of Chemical Physics, 2012, 136, 124104.	3.0	31
96	Continuum Theory of Epitaxial Crystal Growth. I. Journal of Statistical Physics, 2001, 104, 221-253.	1.2	29
97	The Andersen thermostat in molecular dynamics. Communications on Pure and Applied Mathematics, 2008, 61, 96-136.	3.1	29
98	Study of noise-induced transitions in the Lorenz system using the minimum action method. Communications in Mathematical Sciences, 2010, 8, 341-355.	1.0	29
99	A multiscale coupling method for the modeling of dynamics of solids with application to brittle cracks. Journal of Computational Physics, 2010, 229, 3970-3987.	3.8	27
100	A numerical method for the study of nucleation of ordered phases. Journal of Computational Physics, 2010, 229, 1797-1809.	3.8	26
101	The Electronic Structure of Smoothly Deformed Crystals: Wannier Functions and the Cauchy–Born Rule. Archive for Rational Mechanics and Analysis, 2011, 199, 407-433.	2.4	26
102	The Barron Space and the Flow-Induced Function Spaces for Neural Network Models. Constructive Approximation, 2022, 55, 369-406.	3.0	26
103	Probabilistic framework for network partition. Physical Review E, 2009, 80, 026106.	2.1	25
104	The Heterogeneous Multiscale Method Based on the Discontinuous Galerkin Method for Hyperbolic and Parabolic Problems. Multiscale Modeling and Simulation, 2005, 3, 871-894.	1.6	24
105	Machine learning from a continuous viewpoint, I. Science China Mathematics, 2020, 63, 2233-2266.	1.7	24
106	A comparative analysis of optimization and generalization properties of two-layer neural network and random feature models under gradient descent dynamics. Science China Mathematics, 2020, 63, 1235-1258.	1.7	22
107	Gibbsian Dynamics and Invariant Measures for Stochastic Dissipative PDEs. Journal of Statistical Physics, 2002, 108, 1125-1156.	1.2	21
108	Improved gauss-seidel projection method for micromagnetics simulations. IEEE Transactions on Magnetics, 2003, 39, 1766-1770.	2.1	21

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109	Numerical methods for multiscale transport equations and application to two-phase porous media flow. Journal of Computational Physics, 2005, 210, 656-675.	3.8	20
110	Electronic structure of smoothly deformed crystals: Cauchyâ€born rule for the nonlinear tightâ€binding model. Communications on Pure and Applied Mathematics, 2010, 63, 1432-1468.	3.1	20
111	Spatial feedbacks and the dynamics of savanna and forest. Theoretical Ecology, 2019, 12, 237-262.	1.0	20
112	On the distinguished limits of the Navier slip model of the moving contact line problem. Journal of Fluid Mechanics, 2015, 772, 107-126.	3.4	19
113	Can Shallow Neural Networks Beat the Curse of Dimensionality? A Mean Field Training Perspective. IEEE Transactions on Artificial Intelligence, 2020, 1, 121-129.	4.7	19
114	Optimization-Based String Method for Finding Minimum Energy Path. Communications in Computational Physics, 2013, 14, 265-275.	1.7	18
115	Sampling saddle points on a free energy surface. Journal of Chemical Physics, 2014, 140, 164109.	3.0	18
116	A sub-linear scaling algorithm for computing the electronic structure of materials. Communications in Mathematical Sciences, 2007, 5, 999-1026.	1.0	17
117	Correctors for the homogenization of conservation laws with oscillatory forcing terms. Asymptotic Analysis, 1992, 5, 311-316.	0.5	15
118	Theory of phase separation kinetics in polymer–liquid crystal systems. Journal of Chemical Physics, 2002, 116, 4723-4734.	3.0	15
119	Machine-learning-based non-Newtonian fluid model with molecular fidelity. Physical Review E, 2020, 102, 043309.	2.1	15
120	A discontinuous Galerkin implementation of a domain decomposition method for kinetic-hydrodynamic coupling multiscale problems in gas dynamics and device simulations. Journal of Computational Physics, 2007, 225, 1314-1330.	3.8	14
121	Multilevel Picard iterations for solving smooth semilinear parabolic heat equations. SN Partial Differential Equations and Applications, 2021, 2, 1.	0.6	14
122	A continuum model for the growth of epitaxial films. Journal of Crystal Growth, 2001, 222, 414-425.	1.5	13
123	Numerical study of metastability due to tunneling: The quantum string method. Physica A: Statistical Mechanics and Its Applications, 2007, 379, 491-502.	2.6	13
124	Another note on forced burgers turbulence. Physics of Fluids, 2000, 12, 149-154.	4.0	12
125	Convergence of a Stochastic Method for the Modeling of Polymeric Fluids. Acta Mathematicae Applicatae Sinica, 2002, 18, 529-536.	0.7	12
126	A note on generalized flows. Physica D: Nonlinear Phenomena, 2003, 183, 159-174.	2.8	12

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127	Analysis of the Local Quasicontinuum Method. Series in Contemporary Applied Mathematics, 2006, , 18-32.	0.8	12
128	Seamless multiscale modeling via dynamics on fiber bundles. Communications in Mathematical Sciences, 2007, 5, 649-663.	1.0	12
129	Study of the instability of the Poiseuille flow using a thermodynamic formalism. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 9518-9523.	7.1	11
130	Renormalized powers of Ornstein–Uhlenbeck processes and well-posedness of stochastic Ginzburg–Landau equations. Nonlinear Analysis: Theory, Methods & Applications, 2016, 142, 152-193.	1.1	11
131	Adaptive coupling of a deep neural network potential to a classical force field. Journal of Chemical Physics, 2018, 149, 154107.	3.0	11
132	Machine-learning-assisted modeling. Physics Today, 2021, 74, 36-41.	0.3	11
133	Analysis of the heterogeneous multiscale method for gas dynamics. Methods and Applications of Analysis, 2004, 11, 557-572.	0.5	10
134	Density-gradient-corrected embedded atom method. Physical Review B, 2009, 79, .	3.2	9
135	Optimized local basis set for Kohn–Sham density functional theory. Journal of Computational Physics, 2012, 231, 4515-4529.	3.8	9
136	On the statistical solution of the Riemann equation and its implications for Burgers turbulence. Physics of Fluids, 1999, 11, 2149-2153.	4.0	8
137	Subcritical bifurcation in spatially extended systems. Nonlinearity, 2012, 25, 761-779.	1.4	8
138	Kolmogorov width decay and poor approximators in machine learning: shallow neural networks, random feature models and neural tangent kernels. Research in Mathematical Sciences, 2021, 8, 1.	1.0	8
139	The Elastic Continuum Limit of the Tight Binding Model*. Chinese Annals of Mathematics Series B, 2007, 28, 665-676.	0.4	7
140	Asymptotic analysis of quantum dynamics in crystals: the Bloch-Wigner transform, Bloch dynamics and Berry phase. Acta Mathematicae Applicatae Sinica, 2013, 29, 465-476.	0.7	7
141	Effective Maxwell equations from time-dependent density functional theory. Acta Mathematica Sinica, English Series, 2011, 27, 339-368.	0.6	6
142	Efficient iterative method for solving the Dirac–Kohn–Sham density functional theory. Journal of Computational Physics, 2013, 245, 205-217.	3.8	6
143	Multiscale Modeling Of Crystalline Solids. , 2005, , 1491-1506.		5
144	Heterogenous multiscale method for locally self-similar problems. Communications in Mathematical Sciences, 2004, 2, 137-144.	1.0	5

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145	Representation formulas and pointwise properties for Barron functions. Calculus of Variations and Partial Differential Equations, 2022, 61, 1.	1.7	5
146	Domain size in the presence of random fields. Physical Review E, 1998, 57, 135-137.	2.1	4
147	Generalization error of GAN from the discriminator's perspective. Research in Mathematical Sciences, 2022, 9, 1.	1.0	4
148	Coarse-grained spectral projection: A deep learning assisted approach to quantum unitary dynamics. Physical Review B, 2021, 103, .	3.2	3
149	Breakdown of homogenization for the random Hamilton-Jacobi equations. Communications in Mathematical Sciences, 2008, 6, 189-197.	1.0	3
150	Lattice Boltzmann Methods for Multiscale Fluid Problems. , 2005, , 2475-2486.		2
151	Stability and the continuum limit of the spin-polarized Thomas-Fermi-Dirac-von Weizsäker model. Journal of Mathematical Physics, 2012, 53, .	1.1	2
152	The continuum limit and QM-continuum approximation of quantum mechanical models of solids. Communications in Mathematical Sciences, 2007, 5, 679-696.	1.0	2
153	Rademacher complexity and the generalization error of residual networks. Communications in Mathematical Sciences, 2020, 18, 1755-1774.	1.0	2
154	Exact Renormalization Group Analysis of Turbulent Transport by the Shear Flow. Journal of Statistical Physics, 2013, 153, 553-571.	1.2	1
155	The Free Action of Nonequilibrium Dynamics. Journal of Statistical Physics, 2015, 161, 300-325.	1.2	1
156	Machine Learning Approximation Algorithms for High-Dimensional Fully Nonlinear Partial Differential Equations and Second-order Backward Stochastic Differential Equations. , 2019, 29, 1563.		1
157	Probabilistic framework for network partition. , 0, .		1
158	Interface Conditions for Coupled Atomistic and Continuum Models of Solids for Dynamics Problems at Finite Temperature. Materials Research Society Symposia Proceedings, 2006, 978, .	0.1	0
159	A Mathematical Model for Universal Semantics. IEEE Transactions on Pattern Analysis and Machine Intelligence, 2022, 44, 1124-1132.	13.9	0
160	A Priori Estimates of the Generalization Error for Autoencoders. , 2020, , .		0
161	Mathematical theory of solids: From quantum mechanics to continuum models. Discrete and Continuous Dynamical Systems, 2014, 34, 5085-5097.	0.9	0
162	A thermodynamic study of the two-dimensional pressure-driven channel flow. Discrete and Continuous Dynamical Systems, 2016, 36, 4349-4366.	0.9	0

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163	Lattice Boltzmann Methods for Multiscale Fluid Problems. , 2005, , 2475-2486.		0