Michele Ceriotti

List of Publications by Year
in descending order

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169 papers	12,029 citations	26567 56 h-index	29081 104 g-index
172 all docs	172 docs citations	172 times ranked	8846 citing authors

#	Article	IF	Citations
1	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	9.0	655
2	Comparing molecules and solids across structural and alchemical space. Physical Chemistry Chemical Physics, 2016, 18, 13754-13769.	1.3	489
3	Machine learning unifies the modeling of materials and molecules. Science Advances, 2017, 3, e1701816.	4.7	488
4	Nuclear Quantum Effects in Water and Aqueous Systems: Experiment, Theory, and Current Challenges. Chemical Reviews, 2016, 116, 7529-7550.	23.0	439
5	Gaussian Process Regression for Materials and Molecules. Chemical Reviews, 2021, 121, 10073-10141.	23.0	384
6	Nuclear quantum effects enter the mainstream. Nature Reviews Chemistry, 2018, 2, .	13.8	271
7	Simplifying the representation of complex free-energy landscapes using sketch-map. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 13023-13028.	3.3	261
8	Efficient stochastic thermostatting of path integral molecular dynamics. Journal of Chemical Physics, 2010, 133, 124104.	1.2	259
9	Physics-Inspired Structural Representations for Molecules and Materials. Chemical Reviews, 2021, 121, 9759-9815.	23.0	247
10	Automatic selection of atomic fingerprints and reference configurations for machine-learning potentials. Journal of Chemical Physics, 2018, 148, 241730.	1.2	224
11	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	3.0	220
12	Barely porous organic cages for hydrogen isotope separation. Science, 2019, 366, 613-620.	6.0	210
13	Nuclear quantum effects and hydrogen bond fluctuations in water. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 15591-15596.	3.3	204
14	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.	3.3	201
15	Colored-Noise Thermostats Ã la Carte. Journal of Chemical Theory and Computation, 2010, 6, 1170-1180.	2.3	199
16	Origins of structural and electronic transitions in disordered silicon. Nature, 2021, 589, 59-64.	13.7	192
17	i-PI: A Python interface for ab initio path integral molecular dynamics simulations. Computer Physics Communications, 2014, 185, 1019-1026.	3.0	189
18	Nuclear Quantum Effects in Solids Using a Colored-Noise Thermostat. Physical Review Letters, 2009, 103, 030603.	2.9	188

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19	Symmetry-Adapted Machine Learning for Tensorial Properties of Atomistic Systems. Physical Review Letters, 2018, 120, 036002.	2.9	186
20	Transferable Machine-Learning Model of the Electron Density. ACS Central Science, 2019, 5, 57-64.	5.3	178
21	How to remove the spurious resonances from ring polymer molecular dynamics. Journal of Chemical Physics, 2014, 140, 234116.	1.2	174
22	Langevin Equation with Colored Noise for Constant-Temperature Molecular Dynamics Simulations. Physical Review Letters, 2009, 102, 020601.	2.9	170
23	Chemical shifts in molecular solids by machine learning. Nature Communications, 2018, 9, 4501.	5.8	170
24	Machine learning for the structureâ€“energyâ€“property landscapes of molecular crystals. Chemical Science, 2018, 9, 1289-1300.	3.7	153
25	Efficient First-Principles Calculation of the Quantum Kinetic Energy and Momentum Distribution of Nuclei. Physical Review Letters, 2012, 109, 100604.	2.9	151
26	Electrolytes induce long-range orientational order and free energy changes in the H-bond network of bulk water. Science Advances, 2016, 2, e1501891.	4.7	151
27	Using sketch-map coordinates to analyze and bias molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5196-5201.	3.3	147
28	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.	1.2	142
29	Accelerating the convergence of path integral dynamics with a generalized Langevin equation. Journal of Chemical Physics, 2011, 134, 084104.	1.2	139
30	Ab initiostudy of the vibrational properties of crystallineTeO2: TheÎ±,Î², andÎ³phases. Physical Review B, 2006, 73, .	1.1	138
31	Accurate molecular polarizabilities with coupled cluster theory and machine learning. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 3401-3406.	3.3	126
32	Atom-density representations for machine learning. Journal of Chemical Physics, 2019, 150, 154110.	1.2	120
33	Machine Learning Force Fields and Coarse-Grained Variables in Molecular Dynamics: Application to Materials and Biological Systems. Journal of Chemical Theory and Computation, 2020, 16, 4757-4775.	2.3	120
34	A self-learning algorithm for biased molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 17509-17514.	3.3	117
35	Semiconducting Nanowireâ€Based Optoelectronic Fibers. Advanced Materials, 2017, 29, 1700681.	11.1	116
36	Incorporating long-range physics in atomic-scale machine learning. Journal of Chemical Physics, 2019, 151, 204105.	1.2	114

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37	Unsupervised machine learning in atomistic simulations, between predictions and understanding. Journal of Chemical Physics, 2019, 150, 150901.	1.2	113
38	Demonstrating the Transferability and the Descriptive Power of Sketch-Map. Journal of Chemical Theory and Computation, 2013, 9, 1521-1532.	2.3	104
39	Incompleteness of Atomic Structure Representations. Physical Review Letters, 2020, 125, 166001.	2.9	103
40	Fast and Accurate Uncertainty Estimation in Chemical Machine Learning. Journal of Chemical Theory and Computation, 2019, 15, 906-915.	2.3	102
41	Electron density learning of non-covalent systems. Chemical Science, 2019, 10, 9424-9432.	3.7	92
42	Feature optimization for atomistic machine learning yields a data-driven construction of the periodic table of the elements. Physical Chemistry Chemical Physics, 2018, 20, 29661-29668.	1.3	88
43	Gas-sieving zeolitic membranes fabricated by condensation of precursor nanosheets. Nature Materials, 2021, 20, 362-369.	13.3	86
44	Solid-liquid interface free energy through metadynamics simulations. Physical Review B, 2010, 81, .	1.1	84
45	Evidence for supercritical behaviour of high-pressure liquid hydrogen. Nature, 2020, 585, 217-220.	13.7	83
46	Large-Scale Computational Screening of Molecular Organic Semiconductors Using Crystal Structure Prediction. Chemistry of Materials, 2018, 30, 4361-4371.	3.2	79
47	Efficient methods and practical guidelines for simulating isotope effects. Journal of Chemical Physics, 2013, 138, 014112.	1.2	78
48	Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase. Journal of Chemical Physics, 2014, 141, 181101.	1.2	74
49	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	1.0	69
50	Quantum fluctuations and isotope effects in ab initio descriptions of water. Journal of Chemical Physics, 2014, 141, 104502.	1.2	68
51	Predicting molecular dipole moments by combining atomic partial charges and atomic dipoles. Journal of Chemical Physics, 2020, 153, 024113.	1.2	65
52	Direct Measurement of Competing Quantum Effects on the Kinetic Energy of Heavy Water upon Melting. Journal of Physical Chemistry Letters, 2013, 4, 3251-3256.	2.1	64
53	Efficient multiple time scale molecular dynamics: Using colored noise thermostats to stabilize resonances. Journal of Chemical Physics, 2011, 134, 014103.	1.2	61
54	Recognizing molecular patterns by machine learning: An agnostic structural definition of the hydrogen bond. Journal of Chemical Physics, 2014, 141, 174110.	1.2	60

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55	Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol. Physical Review Letters, 2016, 117, 115702.	2.9	59
56	Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods. Journal of Chemical Physics, 2016, 144, 054111.	1.2	58
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.	2.1	57
58	Mapping uncharted territory in iceÂfrom zeolite networks to ice structures. Nature Communications, 2018, 9, 2173.	5.8	57
59	Learning the electronic density of states in condensed matter. Physical Review B, 2020, 102, .	1.1	57
60	Neural network potential for Al-Mg-Si alloys. Physical Review Materials, 2017, 1, .	0.9	57
61	A Surface-Specific Isotope Effect in Mixtures of Light and Heavy Water. Journal of Physical Chemistry C, 2013, 117, 2944-2951.	1.5	55
62	Computing the absolute Gibbs free energy in atomistic simulations: Applications to defects in solids. Physical Review B, 2018, 97, .	1.1	53
63	Fine tuning classical and quantum molecular dynamics using a generalized Langevin equation. Journal of Chemical Physics, 2018, 148, 102301.	1.2	52
64	Probing Defects and Correlations in the Hydrogen-Bond Network of ab Initio Water. Journal of Chemical Theory and Computation, 2016, 12, 1953-1964.	2.3	51
65	Nuclear Quantum Effects in H⁺ and OH^{â€“} Diffusion along Confined Water Wires. Journal of Physical Chemistry Letters, 2016, 7, 3001-3007.	2.1	50
66	The Role of Quantum Effects on Structural and Electronic Fluctuations in Neat and Charged Water. Journal of Physical Chemistry B, 2014, 118, 13226-13235.	1.2	48
67	Uncertainty estimation for molecular dynamics and sampling. Journal of Chemical Physics, 2021, 154, 074102.	1.2	48
68	High order path integrals made easy. Journal of Chemical Physics, 2016, 145, 234103.	1.2	47
69	Recursive evaluation and iterative contraction of N-body equivariant features. Journal of Chemical Physics, 2020, 153, 121101.	1.2	46
70	The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates. Journal of the American Chemical Society, 2012, 134, 8557-8569.	6.6	45
71	Using Gaussian process regression to simulate the vibrational Raman spectra of molecular crystals. New Journal of Physics, 2019, 21, 105001.	1.2	44
72	Nuclear quantum effects inab initiodynamics: Theory and experiments for lithium imide. Physical Review B, 2010, 82, .	1.1	43

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73	Recognizing Local and Global Structural Motifs at the Atomic Scale. Journal of Chemical Theory and Computation, 2018, 14, 486-498.	2.3	43
74	Solid-liquid interfacial free energy out of equilibrium. Physical Review B, 2015, 92, .	1.1	40
75	A Bayesian approach to NMR crystal structure determination. Physical Chemistry Chemical Physics, 2019, 21, 23385-23400.	1.3	39
76	The inefficiency of re-weighted sampling and the curse of system size in high-order path integration. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2012, 468, 2-17.	1.0	37
77	Machine learning meets chemical physics. Journal of Chemical Physics, 2021, 154, 160401.	1.2	37
78	Simulating the ghost: quantum dynamics of the solvated electron. Nature Communications, 2021, 12, 766.	5.8	36
79	Introduction: Machine Learning at the Atomic Scale. Chemical Reviews, 2021, 121, 9719-9721.	23.0	36
80	An efficient and accurate decomposition of the Fermi operator. Journal of Chemical Physics, 2008, 129, 024707.	1.2	35
81	Identifying and Tracking Defects in Dynamic Supramolecular Polymers. Journal of Physical Chemistry B, 2020, 124, 589-599.	1.2	35
82	Multi-scale approach for the prediction of atomic scale properties. Chemical Science, 2021, 12, 2078-2090.	3.7	35
83	Thermally-nucleated self-assembly of water and alcohol into stable structures at hydrophobic interfaces. Nature Communications, 2016, 7, 13064.	5.8	33
84	Decisive role of nuclear quantum effects on surface mediated water dissociation at finite temperature. Journal of Chemical Physics, 2018, 148, 102320.	1.2	32
85	A new kind of atlas of zeolite building blocks. Journal of Chemical Physics, 2019, 151, 154112.	1.2	32
86	Efficient implementation of atom-density representations. Journal of Chemical Physics, 2021, 154, 114109.	1.2	32
87	Assessment of Approximate Methods for Anharmonic Free Energies. Journal of Chemical Theory and Computation, 2019, 15, 5845-5857.	2.3	31
88	Direct path integral estimators for isotope fractionation ratios. Journal of Chemical Physics, 2014, 141, 244112.	1.2	30
89	Generalized convex hull construction for materials discovery. Physical Review Materials, 2018, 2, .	0.9	30
90	Nuclear Quantum Effects in Sodium Hydroxide Solutions from Neural Network Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 10158-10171.	1.2	29

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91	Mapping and classifying molecules from a high-throughput structural database. Journal of Cheminformatics, 2017, 9, 6.	2.8	28
92	Solvent fluctuations and nuclear quantum effects modulate the molecular hyperpolarizability of water. Physical Review B, 2017, 96, .	1.1	28
93	Beyond static structures: Putting forth REMD as a tool to solve problems in computational organic chemistry. Journal of Computational Chemistry, 2016, 37, 83-92.	1.5	27
94	Approximating Matsubara dynamics using the planetary model: Tests on liquid water and ice. Journal of Chemical Physics, 2018, 148, 102336.	1.2	27
95	Hydrogen Diffusion and Trapping in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Iron: The Role of Quantum and Anharmonic Fluctuations. Physical Review Letters, 2018, 120, 225901.	2.9	26
96	Simulating Solvation and Acidity in Complex Mixtures with First-Principles Accuracy: The Case of CH₃SO₃H and H₂O₂ in Phenol. Journal of Chemical Theory and Computation, 2020, 16, 5139-5149.	2.3	26
97	Inexpensive modeling of quantum dynamics using path integral generalized Langevin equation thermostats. Journal of Chemical Physics, 2020, 152, 124104.	1.2	26
98	Structure-property maps with Kernel principal covariates regression. Machine Learning: Science and Technology, 2020, 1, 045021.	2.4	26
99	Equivariant representations for molecular Hamiltonians and N-center atomic-scale properties. Journal of Chemical Physics, 2022, 156, 014115.	1.2	26
100	Probing the Unfolded Configurations of a Î²-Hairpin Using Sketch-Map. Journal of Chemical Theory and Computation, 2015, 11, 1086-1093.	2.3	25
101	Accelerated path integral methods for atomistic simulations at ultra-low temperatures. Journal of Chemical Physics, 2016, 145, 054101.	1.2	25
102	Second-Harmonic Scattering as a Probe of Structural Correlations in Liquids. Journal of Physical Chemistry Letters, 2016, 7, 4311-4316.	2.1	25
103	Theoretical prediction of the homogeneous ice nucleation rate: disentangling thermodynamics and kinetics. Physical Chemistry Chemical Physics, 2018, 20, 28732-28740.	1.3	25
104	The role of feature space in atomistic learning. Machine Learning: Science and Technology, 2021, 2, 025028.	2.4	25
105	Learning Electron Densities in the Condensed Phase. Journal of Chemical Theory and Computation, 2021, 17, 7203-7214.	2.3	24
106	Diffusion and desorption of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Si</mml:mi><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>on hydrogenated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">H</mml:mi><mml:mo>:</mml:mo><mml:mi mathvariant="normal">Si</mml:mi><	1.1	23
107	Improving sample and feature selection with principal covariates regression. Machine Learning: Science and Technology, 2021, 2, 035038.	2.4	23
108	Communication: Mean-field theory of water-water correlations in electrolyte solutions. Journal of Chemical Physics, 2017, 146, .	1.2	22

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109	Modeling the Structural and Thermal Properties of Loaded Metalâ€“Organic Frameworks. An Interplay of Quantum and Anharmonic Fluctuations. Journal of Chemical Theory and Computation, 2019, 15, 3237-3249.	2.3	22
110	First principles study of Geâ•Si exchange mechanisms at the Si(001) surface. Applied Physics Letters, 2008, 92, 191908.	1.5	21
111	Quantum mechanical static dipole polarizabilities in the QM7b and AlphaML showcase databases. Scientific Data, 2019, 6, 152.	2.4	20
112	Finite-temperature materials modeling from the quantum nuclei to the hot electron regime. Physical Review Materials, 2021, 5, .	0.9	20
113	Bridging the gap between atomistic and macroscopic models of homogeneous nucleation. Journal of Chemical Physics, 2017, 146, 034106.	1.2	19
114	Understanding How Ligand Functionalization Influences CO2 and N2 Adsorption in a Sodalite Metalâ€“Organic Framework. Chemistry of Materials, 2020, 32, 1526-1536.	3.2	19
115	Quantitative estimate of H abstraction by thermalSiH3on hydrogenatedSi(001)(2Ã—1). Physical Review B, 2007, 75, .	1.1	18
116	The <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mi>Î´</mml:mi></mml:math>-thermostat: selective normal-modes excitation by colored-noise Langevin dynamics. Procedia Computer Science, 2010, 1, 1607-1614.	1.2	18
117	Simulating Energy Relaxation in Pumpâ€“Probe Vibrational Spectroscopy of Hydrogen-Bonded Liquids. Journal of Chemical Theory and Computation, 2017, 13, 1284-1292.	2.3	18
118	Machine learning for metallurgy III: A neural network potential for Al-Mg-Si. Physical Review Materials, 2021, 5, .	0.9	17
119	Optimal radial basis for density-based atomic representations. Journal of Chemical Physics, 2021, 155, 104106.	1.2	17
120	Effects of High Angular Momentum on the Unimolecular Dissociation of CD2CD2OH: Theory and Comparisons with Experiment. Journal of Physical Chemistry A, 2013, 117, 10951-10963.	1.1	16
121	Chemiscope: interactive structure-property explorer for materials and molecules. Journal of Open Source Software, 2020, 5, 2117.	2.0	16
122	An Inâ€Situ Neutron Diffraction and DFT Study of Hydrogen Adsorption in a Sodaliteâ€Type Metalâ€“Organic Framework, Cuâ€BTTri. European Journal of Inorganic Chemistry, 2019, 2019, 1147-1154.	1.0	15
123	Unified theory of atom-centered representations and message-passing machine-learning schemes. Journal of Chemical Physics, 2022, 156, .	1.2	15
124	Ab initiostudy of the diffusion and decomposition pathways of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiH</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub> on Si(100). Physical Review B, 2009, 79, .	1.1	14
125	Ab initio modelling of the early stages of precipitation in Al-6000 alloys. Acta Materialia, 2017, 140, 240-249.	3.8	14
126	Iterative Unbiasing of Quasi-Equilibrium Sampling. Journal of Chemical Theory and Computation, 2020, 16, 100-107.	2.3	14

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127	Modeling the Ga/As binary system across temperatures and compositions from first principles. Physical Review Materials, 2021, 5, .	0.9	14
128	Bayesian probabilistic assignment of chemical shifts in organic solids. Science Advances, 2021, 7, eabk2341.	4.7	13
129	Static disorder and structural correlations in the low-temperature phase of lithium imide. Physical Review B, 2011, 83, .	1.1	12
130	Communication: Computing the Tolman length for solid-liquid interfaces. Journal of Chemical Physics, 2018, 148, 231102.	1.2	12
131	Anisotropy of the Proton Momentum Distribution in Water. Journal of Physical Chemistry B, 2018, 122, 6048-6054.	1.2	12
132	Atomic-Scale Representation and Statistical Learning of Tensorial Properties. ACS Symposium Series, 2019, , 1-21.	0.5	12
133	Global Free-Energy Landscapes as a Smoothly Joined Collection of Local Maps. Journal of Chemical Theory and Computation, 2021, 17, 3292-3308.	2.3	12
134	Quantum vibronic effects on the electronic properties of solid and molecular carbon. Physical Review Materials, 2021, 5, .	0.9	12
135	A Hybrid Approach to Fermi Operator Expansion. , 2009, , .		11
136	Simultaneous measurement of lithium and fluorine momentum in⁷LiF. Journal of Physics Condensed Matter, 2012, 24, 365401.	0.7	11
137	Mapping the conformational free energy of aspartic acid in the gas phase and in aqueous solution. Journal of Chemical Physics, 2017, 146, 145102.	1.2	10
138	The Gibbs free energy of homogeneous nucleation: From atomistic nuclei to the planar limit. Journal of Chemical Physics, 2017, 147, 104707.	1.2	10
139	Energy Relaxation and Thermal Diffusion in Infrared Pumpâ€“Probe Spectroscopy of Hydrogen-Bonded Liquids. Journal of Physical Chemistry Letters, 2019, 10, 3447-3452.	2.1	10
140	Atomic Motif Recognition in (Bio)Polymers: Benchmarks From the Protein Data Bank. Frontiers in Molecular Biosciences, 2019, 6, 24.	1.6	10
141	3D Ordering at the Liquidâ€“Solid Polar Interface of Nanowires. Advanced Materials, 2020, 32, e2001030.	11.1	10
142	Importance of Nuclear Quantum Effects for NMR Crystallography. Journal of Physical Chemistry Letters, 2021, 12, 7701-7707.	2.1	9
143	Local invertibility and sensitivity of atomic structure-feature mappings. Open Research Europe, 0, 1, 126.	2.0	9
144	Determination and evaluation of the nonadditivity in wetting of molecularly heterogeneous surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 25516-25523.	3.3	8

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145	Local Kernel Regression and Neural Network Approaches to the Conformational Landscapes of Oligopeptides. Journal of Chemical Theory and Computation, 2022, 18, 1467-1479.	2.3	8
146	First-Principles Study of the High-Temperature Phase of Li₂NH. Journal of Physical Chemistry C, 2011, 115, 7076-7080.	1.5	7
147	Accurate Description of Nuclear Quantum Effects with High-Order Perturbed Path Integrals (HOPPI). Journal of Chemical Theory and Computation, 2020, 16, 1128-1135.	2.3	7
148	Classical nucleation theory predicts the shape of the nucleus in homogeneous solidification. Journal of Chemical Physics, 2020, 152, 044103.	1.2	7
149	Impact-driven effects in thin-film growth: steering and transient mobility at the Ag(110) surface. Nanotechnology, 2006, 17, 3556-3562.	1.3	6
150	Extracting the interfacial free energy and anisotropy from a smooth fluctuating dividing surface. Journal of Physics Condensed Matter, 2017, 29, 445001.	0.7	6
151	Machine Learning of Atomic-Scale Properties Based on Physical Principles. , 2018, , 1-27.		6
152	Fast-forward Langevin dynamics with momentum flips. Journal of Chemical Physics, 2018, 148, 184109.	1.2	6
153	Quantum kinetic energy and isotope fractionation in aqueous ionic solutions. Physical Chemistry Chemical Physics, 2020, 22, 10490-10499.	1.3	6
154	Analyzing Fluxional Molecules Using DORI. Journal of Chemical Theory and Computation, 2018, 14, 2370-2379.	2.3	5
155	Evaluating functions of positive-definite matrices using colored-noise thermostats. Physical Review E, 2014, 89, 023302.	0.8	4
156	Discussion: Measurement and Instrumentation. Journal of Physics: Conference Series, 2014, 571, 012010.	0.3	4
157	Machine Learning at the Atomic Scale. Chimia, 2019, 73, 972.	0.3	4
158	Machine-Learning of Atomic-Scale Properties Based on Physical Principles. Lecture Notes in Physics, 2020, , 99-127.	0.3	4
159	Discussion: Nuclear Quantum Dynamics - Protons and Beyond. Journal of Physics: Conference Series, 2014, 571, 012004.	0.3	3
160	Discussion: Theoretical Horizons and Calculation. Journal of Physics: Conference Series, 2014, 571, 012013.	0.3	3
161	Comment on â€œWater-water correlations in electrolyte solutions probed by hyper-Rayleigh scatteringâ€• [J. Chem. Phys. 147, 214505 (2017)]. Journal of Chemical Physics, 2018, 149, 167101.	1.2	3
162	Machine Learning of Atomic-Scale Properties Based on Physical Principles. , 2020, , 1911-1937.		3

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163	Conjugate gradient heat bath for ill-conditioned actions. Physical Review E, 2007, 76, 026707.	0.8	2
164	Density functional study of the decomposition pathways of SiH₃and GeH₃at the Si(100) and Ge(100) surfaces. Journal of Physics Condensed Matter, 2012, 24, 104002.	0.7	2
165	Chemical physics software. Journal of Chemical Physics, 2021, 155, 010401.	1.2	2
166	Reply to: On the liquidâ€“liquid phase transition of dense hydrogen. Nature, 2021, 600, E15-E16.	13.7	2
167	Ab initio simulation of particle momentum distributions in high-pressure water. Journal of Physics: Conference Series, 2014, 571, 012011.	0.3	1
168	Machines learn to recognize glasses. Nature Physics, 2016, 12, 377-378.	6.5	1
169	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	1.2	1