Michele Ceriotti

List of Publications by Year
in descending order

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169	12,029	26630 56	29157 104
papers	citations	h-index	g-index

172	172	172	8846
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Equivariant representations for molecular Hamiltonians and N-center atomic-scale properties. Journal of Chemical Physics, 2022, 156, 014115.	3.0	26
2	Local Kernel Regression and Neural Network Approaches to the Conformational Landscapes of Oligopeptides. Journal of Chemical Theory and Computation, 2022, 18, 1467-1479.	5.3	8
3	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	2.8	69
4	Unified theory of atom-centered representations and message-passing machine-learning schemes. Journal of Chemical Physics, 2022, 156, .	3.0	15
5	Gas-sieving zeolitic membranes fabricated by condensation of precursor nanosheets. Nature Materials, 2021, 20, 362-369.	27.5	86
6	Multi-scale approach for the prediction of atomic scale properties. Chemical Science, 2021, 12, 2078-2090.	7.4	35
7	Origins of structural and electronic transitions in disordered silicon. Nature, 2021, 589, 59-64.	27.8	192
8	Uncertainty estimation for molecular dynamics and sampling. Journal of Chemical Physics, 2021, 154, 074102.	3.0	48
9	Simulating the ghost: quantum dynamics of the solvated electron. Nature Communications, 2021, 12, 766.	12.8	36
10	Efficient implementation of atom-density representations. Journal of Chemical Physics, 2021, 154, 114109.	3.0	32
11	The role of feature space in atomistic learning. Machine Learning: Science and Technology, 2021, 2, 025028.	5.0	25
12	Finite-temperature materials modeling from the quantum nuclei to the hot electron regime. Physical Review Materials, 2021, 5, .	2.4	20
13	Machine learning meets chemical physics. Journal of Chemical Physics, 2021, 154, 160401.	3.0	37
14	Machine learning for metallurgy III: A neural network potential for Al-Mg-Si. Physical Review Materials, 2021, 5, .	2.4	17
15	Global Free-Energy Landscapes as a Smoothly Joined Collection of Local Maps. Journal of Chemical Theory and Computation, 2021, 17, 3292-3308.	5.3	12
16	Modeling the Ga/As binary system across temperatures and compositions from first principles. Physical Review Materials, 2021, 5, .	2.4	14
17	Improving sample and feature selection with principal covariates regression. Machine Learning: Science and Technology, 2021, 2, 035038.	5.0	23
18	Quantum vibronic effects on the electronic properties of solid and molecular carbon. Physical Review Materials, 2021, 5, .	2.4	12

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19	Physics-Inspired Structural Representations for Molecules and Materials. Chemical Reviews, 2021, 121, 9759-9815.	47.7	247
20	Chemical physics software. Journal of Chemical Physics, 2021, 155, 010401.	3.0	2
21	Introduction: Machine Learning at the Atomic Scale. Chemical Reviews, 2021, 121, 9719-9721.	47.7	36
22	Importance of Nuclear Quantum Effects for NMR Crystallography. Journal of Physical Chemistry Letters, 2021, 12, 7701-7707.	4.6	9
23	Gaussian Process Regression for Materials and Molecules. Chemical Reviews, 2021, 121, 10073-10141.	47.7	384
24	Optimal radial basis for density-based atomic representations. Journal of Chemical Physics, 2021, 155, 104106.	3.0	17
25	Learning Electron Densities in the Condensed Phase. Journal of Chemical Theory and Computation, 2021, 17, 7203-7214.	5.3	24
26	Bayesian probabilistic assignment of chemical shifts in organic solids. Science Advances, 2021, 7, eabk2341.	10.3	13
27	Reply to: On the liquidâ€“liquid phase transition of dense hydrogen. Nature, 2021, 600, E15-E16.	27.8	2
28	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	3.0	1
29	Accurate Description of Nuclear Quantum Effects with High-Order Perturbed Path Integrals (HOPPI). Journal of Chemical Theory and Computation, 2020, 16, 1128-1135.	5.3	7
30	Identifying and Tracking Defects in Dynamic Supramolecular Polymers. Journal of Physical Chemistry B, 2020, 124, 589-599.	2.6	35
31	Iterative Unbiasing of Quasi-Equilibrium Sampling. Journal of Chemical Theory and Computation, 2020, 16, 100-107.	5.3	14
32	Recursive evaluation and iterative contraction of N-body equivariant features. Journal of Chemical Physics, 2020, 153, 121101.	3.0	46
33	Incompleteness of Atomic Structure Representations. Physical Review Letters, 2020, 125, 166001.	7.8	103
34	Predicting molecular dipole moments by combining atomic partial charges and atomic dipoles. Journal of Chemical Physics, 2020, 153, 024113.	3.0	65
35	3D Ordering at the Liquidâ€“Solid Polar Interface of Nanowires. Advanced Materials, 2020, 32, e2001030.	21.0	10
36	Evidence for supercritical behaviour of high-pressure liquid hydrogen. Nature, 2020, 585, 217-220.	27.8	83

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37	Learning the electronic density of states in condensed matter. Physical Review B, 2020, 102, .	3.2	57
38	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.	5.3	26
39	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.	5.3	120
40	Inexpensive modeling of quantum dynamics using path integral generalized Langevin equation thermostats. Journal of Chemical Physics, 2020, 152, 124104.	3.0	26
41	Quantum kinetic energy and isotope fractionation in aqueous ionic solutions. Physical Chemistry Chemical Physics, 2020, 22, 10490-10499.	2.8	6
42	Classical nucleation theory predicts the shape of the nucleus in homogeneous solidification. Journal of Chemical Physics, 2020, 152, 044103.	3.0	7
43	Understanding How Ligand Functionalization Influences CO2 and N2 Adsorption in a Sodalite Metalâ€“Organic Framework. Chemistry of Materials, 2020, 32, 1526-1536.	6.7	19
44	Machine-Learning of Atomic-Scale Properties Based on Physical Principles. Lecture Notes in Physics, 2020, , 99-127.	0.7	4
45	Machine Learning of Atomic-Scale Properties Based on Physical Principles. , 2020, , 1911-1937.		3
46	Structure-property maps with Kernel principal covariates regression. Machine Learning: Science and Technology, 2020, 1, 045021.	5.0	26
47	Chemiscope: interactive structure-property explorer for materials and molecules. Journal of Open Source Software, 2020, 5, 2117.	4.6	16
48	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
49	Using Gaussian process regression to simulate the vibrational Raman spectra of molecular crystals. New Journal of Physics, 2019, 21, 105001.	2.9	44
50	Barely porous organic cages for hydrogen isotope separation. Science, 2019, 366, 613-620.	12.6	210
51	A new kind of atlas of zeolite building blocks. Journal of Chemical Physics, 2019, 151, 154112.	3.0	32
52	Electron density learning of non-covalent systems. Chemical Science, 2019, 10, 9424-9432.	7.4	92
53	Quantum mechanical static dipole polarizabilities in the QM7b and AlphaML showcase databases. Scientific Data, 2019, 6, 152.	5.3	20
54	Assessment of Approximate Methods for Anharmonic Free Energies. Journal of Chemical Theory and Computation, 2019, 15, 5845-5857.	5.3	31

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55	Energy Relaxation and Thermal Diffusion in Infrared Pumpâ€“Probe Spectroscopy of Hydrogen-Bonded Liquids. Journal of Physical Chemistry Letters, 2019, 10, 3447-3452.	4.6	10
56	Atomic Motif Recognition in (Bio)Polymers: Benchmarks From the Protein Data Bank. Frontiers in Molecular Biosciences, 2019, 6, 24.	3.5	10
57	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.	5.3	22
58	Atom-density representations for machine learning. Journal of Chemical Physics, 2019, 150, 154110.	3.0	120
59	Unsupervised machine learning in atomistic simulations, between predictions and understanding. Journal of Chemical Physics, 2019, 150, 150901.	3.0	113
60	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.	7.1	126
61	Incorporating long-range physics in atomic-scale machine learning. Journal of Chemical Physics, 2019, 151, 204105.	3.0	114
62	Atomic-Scale Representation and Statistical Learning of Tensorial Properties. ACS Symposium Series, 2019, , 1-21.	0.5	12
63	Machine Learning at the Atomic Scale. Chimia, 2019, 73, 972.	0.6	4
64	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.	7.1	8
65	A Bayesian approach to NMR crystal structure determination. Physical Chemistry Chemical Physics, 2019, 21, 23385-23400.	2.8	39
66	Transferable Machine-Learning Model of the Electron Density. ACS Central Science, 2019, 5, 57-64.	11.3	178
67	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.	7.1	201
68	Fast and Accurate Uncertainty Estimation in Chemical Machine Learning. Journal of Chemical Theory and Computation, 2019, 15, 906-915.	5.3	102
69	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.	2.0	15
70	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	7.5	220
71	Nuclear quantum effects enter the mainstream. Nature Reviews Chemistry, 2018, 2, .	30.2	271
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.	3.0	142

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73	Computing the absolute Gibbs free energy in atomistic simulations: Applications to defects in solids. Physical Review B, 2018, 97, .	3.2	53
74	Decisive role of nuclear quantum effects on surface mediated water dissociation at finite temperature. Journal of Chemical Physics, 2018, 148, 102320.	3.0	32
75	Symmetry-Adapted Machine Learning for Tensorial Properties of Atomistic Systems. Physical Review Letters, 2018, 120, 036002.	7.8	186
76	Recognizing Local and Global Structural Motifs at the Atomic Scale. Journal of Chemical Theory and Computation, 2018, 14, 486-498.	5.3	43
77	Approximating Matsubara dynamics using the planetary model: Tests on liquid water and ice. Journal of Chemical Physics, 2018, 148, 102336.	3.0	27
78	Analyzing Fluxional Molecules Using DORI. Journal of Chemical Theory and Computation, 2018, 14, 2370-2379.	5.3	5
79	Fine tuning classical and quantum molecular dynamics using a generalized Langevin equation. Journal of Chemical Physics, 2018, 148, 102301.	3.0	52
80	Machine learning for the structureâ€“energyâ€“property landscapes of molecular crystals. Chemical Science, 2018, 9, 1289-1300.	7.4	153
81	Theoretical prediction of the homogeneous ice nucleation rate: disentangling thermodynamics and kinetics. Physical Chemistry Chemical Physics, 2018, 20, 28732-28740.	2.8	25
82	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.	2.8	88
83	Machine Learning of Atomic-Scale Properties Based on Physical Principles. , 2018, , 1-27.		6
84	Nuclear Quantum Effects in Sodium Hydroxide Solutions from Neural Network Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 10158-10171.	2.6	29
85	Chemical shifts in molecular solids by machine learning. Nature Communications, 2018, 9, 4501.	12.8	170
86	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.	3.0	3
87	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.	7.8	26
88	Automatic selection of atomic fingerprints and reference configurations for machine-learning potentials. Journal of Chemical Physics, 2018, 148, 241730.	3.0	224
89	Fast-forward Langevin dynamics with momentum flips. Journal of Chemical Physics, 2018, 148, 184109.	3.0	6
90	Communication: Computing the Tolman length for solid-liquid interfaces. Journal of Chemical Physics, 2018, 148, 231102.	3.0	12

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91	Anisotropy of the Proton Momentum Distribution in Water. Journal of Physical Chemistry B, 2018, 122, 6048-6054.	2.6	12
92	Mapping uncharted territory in iceÂfrom zeolite networks to ice structures. Nature Communications, 2018, 9, 2173.	12.8	57
93	Large-Scale Computational Screening of Molecular Organic Semiconductors Using Crystal Structure Prediction. Chemistry of Materials, 2018, 30, 4361-4371.	6.7	79
94	Generalized convex hull construction for materials discovery. Physical Review Materials, 2018, 2, .	2.4	30
95	Simulating Energy Relaxation in Pumpâ€“Probe Vibrational Spectroscopy of Hydrogen-Bonded Liquids. Journal of Chemical Theory and Computation, 2017, 13, 1284-1292.	5.3	18
96	Mapping and classifying molecules from a high-throughput structural database. Journal of Cheminformatics, 2017, 9, 6.	6.1	28
97	Bridging the gap between atomistic and macroscopic models of homogeneous nucleation. Journal of Chemical Physics, 2017, 146, 034106.	3.0	19
98	Mapping the conformational free energy of aspartic acid in the gas phase and in aqueous solution. Journal of Chemical Physics, 2017, 146, 145102.	3.0	10
99	Semiconducting Nanowireâ€Based Optoelectronic Fibers. Advanced Materials, 2017, 29, 1700681.	21.0	116
100	Communication: Mean-field theory of water-water correlations in electrolyte solutions. Journal of Chemical Physics, 2017, 146, .	3.0	22
101	Solvent fluctuations and nuclear quantum effects modulate the molecular hyperpolarizability of water. Physical Review B, 2017, 96, .	3.2	28
102	The Gibbs free energy of homogeneous nucleation: From atomistic nuclei to the planar limit. Journal of Chemical Physics, 2017, 147, 104707.	3.0	10
103	Ab initio modelling of the early stages of precipitation in Al-6000 alloys. Acta Materialia, 2017, 140, 240-249.	7.9	14
104	Machine learning unifies the modeling of materials and molecules. Science Advances, 2017, 3, e1701816.	10.3	488
105	Extracting the interfacial free energy and anisotropy from a smooth fluctuating dividing surface. Journal of Physics Condensed Matter, 2017, 29, 445001.	1.8	6
106	Neural network potential for Al-Mg-Si alloys. Physical Review Materials, 2017, 1, .	2.4	57
107	High order path integrals made easy. Journal of Chemical Physics, 2016, 145, 234103.	3.0	47
108	Accelerated path integral methods for atomistic simulations at ultra-low temperatures. Journal of Chemical Physics, 2016, 145, 054101.	3.0	25

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109	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.	3.0	58
110	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.	4.6	57
111	Nuclear Quantum Effects in Water and Aqueous Systems: Experiment, Theory, and Current Challenges. Chemical Reviews, 2016, 116, 7529-7550.	47.7	439
112	Comparing molecules and solids across structural and alchemical space. Physical Chemistry Chemical Physics, 2016, 18, 13754-13769.	2.8	489
113	Machines learn to recognize glasses. Nature Physics, 2016, 12, 377-378.	16.7	1
114	Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol. Physical Review Letters, 2016, 117, 115702.	7.8	59
115	Second-Harmonic Scattering as a Probe of Structural Correlations in Liquids. Journal of Physical Chemistry Letters, 2016, 7, 4311-4316.	4.6	25
116	Nuclear Quantum Effects in H⁺ and OH^{â€“} Diffusion along Confined Water Wires. Journal of Physical Chemistry Letters, 2016, 7, 3001-3007.	4.6	50
117	Electrolytes induce long-range orientational order and free energy changes in the H-bond network of bulk water. Science Advances, 2016, 2, e1501891.	10.3	151
118	Thermally-nucleated self-assembly of water and alcohol into stable structures at hydrophobic interfaces. Nature Communications, 2016, 7, 13064.	12.8	33
119	Beyond static structures: Putting forth REMD as a tool to solve problems in computational organic chemistry. Journal of Computational Chemistry, 2016, 37, 83-92.	3.3	27
120	Probing Defects and Correlations in the Hydrogen-Bond Network of ab Initio Water. Journal of Chemical Theory and Computation, 2016, 12, 1953-1964.	5.3	51
121	Solid-liquid interfacial free energy out of equilibrium. Physical Review B, 2015, 92, .	3.2	40
122	Probing the Unfolded Configurations of a Î²-Hairpin Using Sketch-Map. Journal of Chemical Theory and Computation, 2015, 11, 1086-1093.	5.3	25
123	Discussion: Nuclear Quantum Dynamics - Protons and Beyond. Journal of Physics: Conference Series, 2014, 571, 012004.	0.4	3
124	Direct path integral estimators for isotope fractionation ratios. Journal of Chemical Physics, 2014, 141, 244112.	3.0	30
125	Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase. Journal of Chemical Physics, 2014, 141, 181101.	3.0	74
126	Recognizing molecular patterns by machine learning: An agnostic structural definition of the hydrogen bond. Journal of Chemical Physics, 2014, 141, 174110.	3.0	60

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127	How to remove the spurious resonances from ring polymer molecular dynamics. Journal of Chemical Physics, 2014, 140, 234116.	3.0	174
128	Quantum fluctuations and isotope effects in ab initio descriptions of water. Journal of Chemical Physics, 2014, 141, 104502.	3.0	68
129	The Role of Quantum Effects on Structural and Electronic Fluctuations in Neat and Charged Water. Journal of Physical Chemistry B, 2014, 118, 13226-13235.	2.6	48
130	Evaluating functions of positive-definite matrices using colored-noise thermostats. Physical Review E, 2014, 89, 023302.	2.1	4
131	i-PI: A Python interface for ab initio path integral molecular dynamics simulations. Computer Physics Communications, 2014, 185, 1019-1026.	7.5	189
132	Ab initio simulation of particle momentum distributions in high-pressure water. Journal of Physics: Conference Series, 2014, 571, 012011.	0.4	1
133	Discussion: Measurement and Instrumentation. Journal of Physics: Conference Series, 2014, 571, 012010.	0.4	4
134	Discussion: Theoretical Horizons and Calculation. Journal of Physics: Conference Series, 2014, 571, 012013.	0.4	3
135	A Surface-Specific Isotope Effect in Mixtures of Light and Heavy Water. Journal of Physical Chemistry C, 2013, 117, 2944-2951.	3.1	55
136	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.	2.5	16
137	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.	7.1	204
138	Demonstrating the Transferability and the Descriptive Power of Sketch-Map. Journal of Chemical Theory and Computation, 2013, 9, 1521-1532.	5.3	104
139	Direct Measurement of Competing Quantum Effects on the Kinetic Energy of Heavy Water upon Melting. Journal of Physical Chemistry Letters, 2013, 4, 3251-3256.	4.6	64
140	Efficient methods and practical guidelines for simulating isotope effects. Journal of Chemical Physics, 2013, 138, 014112.	3.0	78
141	Simultaneous measurement of lithium and fluorine momentum in⁷LiF. Journal of Physics Condensed Matter, 2012, 24, 365401.	1.8	11
142	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.	1.8	2
143	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.	7.1	147
144	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.	2.1	37

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145	Efficient First-Principles Calculation of the Quantum Kinetic Energy and Momentum Distribution of Nuclei. Physical Review Letters, 2012, 109, 100604.	7.8	151
146	The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates. Journal of the American Chemical Society, 2012, 134, 8557-8569.	13.7	45
147	Accelerating the convergence of path integral dynamics with a generalized Langevin equation. Journal of Chemical Physics, 2011, 134, 084104.	3.0	139
148	Static disorder and structural correlations in the low-temperature phase of lithium imide. Physical Review B, 2011, 83, .	3.2	12
149	First-Principles Study of the High-Temperature Phase of Li₂NH. Journal of Physical Chemistry C, 2011, 115, 7076-7080.	3.1	7
150	Efficient multiple time scale molecular dynamics: Using colored noise thermostats to stabilize resonances. Journal of Chemical Physics, 2011, 134, 014103.	3.0	61
151	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.	7.1	261
152	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.	2.0	18
153	Nuclear quantum effects inab initiodynamics: Theory and experiments for lithium imide. Physical Review B, 2010, 82, .	3.2	43
154	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.	7.1	117
155	Colored-Noise Thermostats Ã la Carte. Journal of Chemical Theory and Computation, 2010, 6, 1170-1180.	5.3	199
156	Efficient stochastic thermostatting of path integral molecular dynamics. Journal of Chemical Physics, 2010, 133, 124104.	3.0	259
157	Solid-liquid interface free energy through metadynamics simulations. Physical Review B, 2010, 81, .	3.2	84
158	A Hybrid Approach to Fermi Operator Expansion. , 2009, , .		11
159	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, .	3.2	14
160	Langevin Equation with Colored Noise for Constant-Temperature Molecular Dynamics Simulations. Physical Review Letters, 2009, 102, 020601.	7.8	170
161	Nuclear Quantum Effects in Solids Using a Colored-Noise Thermostat. Physical Review Letters, 2009, 103, 030603.	7.8	188
162	An efficient and accurate decomposition of the Fermi operator. Journal of Chemical Physics, 2008, 129, 024707.	3.0	35

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163	First principles study of Geâ^•Si exchange mechanisms at the Si(001) surface. Applied Physics Letters, 2008, 92, 191908.	3.3	21
164	Quantitative estimate of H abstraction by thermalSiH3on hydrogenatedSi(001)(2Ã—1). Physical Review B, 2007, 75, .	3.2	18
165	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></	3.2	23
166	Conjugate gradient heat bath for ill-conditioned actions. Physical Review E, 2007, 76, 026707.	2.1	2
167	Ab initiostudy of the vibrational properties of crystallineTeO2: Theîł,Î², andÎ³phases. Physical Review B, 2006, 73, .	3.2	138
168	Impact-driven effects in thin-film growth: steering and transient mobility at the Ag(110) surface. Nanotechnology, 2006, 17, 3556-3562.	2.6	6
169	Local invertibility and sensitivity of atomic structure-feature mappings. Open Research Europe, 0, 1, 126.	2.0	9