Michele Parrinello

List of Publications by Year
in descending order

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449	102,369	668 122	220 308
papers	citations	h-index	g-index

466	466	466	50609
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Using metadynamics to build neural network potentials for reactive events: the case of urea decomposition in water. Catalysis Today, 2022, 387, 143-149.	4.4	57
2	Breviarium de Motu Simulato Ad Atomos Pertinenti. Israel Journal of Chemistry, 2022, 62, .	2.3	3
3	Prediction of a Supersolid Phase in High-Pressure Deuterium. Physical Review Letters, 2022, 128, 045301.	7.8	16
4	Discover, Sample, and Refine: Exploring Chemistry with Enhanced Sampling Techniques. Journal of Physical Chemistry Letters, 2022, 13, 1424-1430.	4.6	12
5	Computing Rates and Understanding Unbinding Mechanisms in Hostâ€“Guest Systems. Journal of Chemical Theory and Computation, 2022, 18, 1314-1319.	5.3	4
6	Exploration vs Convergence Speed in Adaptive-Bias Enhanced Sampling. Journal of Chemical Theory and Computation, 2022, 18, 3988-3996.	5.3	30
7	Solubility of Organic Salts in Solventâ€“Antisolvent Mixtures: A Combined Experimental and Molecular Dynamics Simulations Approach. Journal of Chemical Theory and Computation, 2022, 18, 4952-4959.	5.3	3
8	The role of water in host-guest interaction. Nature Communications, 2021, 12, 93.	12.8	37
9	Collective variables for the study of crystallisation. Molecular Physics, 2021, 119, .	1.7	25
10	A combined molecular dynamics and experimental study of two-step process enabling low-temperature formation of phase-pure Î±-FAPbI ₃. Science Advances, 2021, 7, .	10.3	49
11	Confinement effects and acid strength in zeolites. Nature Communications, 2021, 12, 2630.	12.8	90
12	Solubility Prediction of Organic Molecules with Molecular Dynamics Simulations. Crystal Growth and Design, 2021, 21, 5198-5205.	3.0	14
13	A modified nudged elastic band algorithm with adaptive spring lengths. Journal of Chemical Physics, 2021, 155, 074103.	3.0	0
14	Water-Triggered, Irreversible Conformational Change of SARS-CoV-2 Main Protease on Passing from the Solid State to Aqueous Solution. Journal of the American Chemical Society, 2021, 143, 12930-12934.	13.7	13
15	Liquid-Liquid Critical Point in Phosphorus. Physical Review Letters, 2021, 127, 080603.	7.8	28
16	From Enhanced Sampling to Reaction Profiles. Journal of Physical Chemistry Letters, 2021, 12, 8621-8626.	4.6	16
17	Targeted Free Energy Perturbation Revisited: Accurate Free Energies from Mapped Reference Potentials. Journal of Physical Chemistry Letters, 2021, 12, 9449-9454.	4.6	15
18	Deep learning the slow modes for rare events sampling. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	104

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19	A metadynamics perspective on the reduction mechanism of the Pt(IV) asplatin prodrug. Journal of Computational Chemistry, 2020, 41, 290-294.	3.3	3
20	Atomistic Mechanism of the Nucleation of Methylammonium Lead Iodide Perovskite from Solution. Chemistry of Materials, 2020, 32, 529-536.	6.7	45
21	Accuracy of Molecular Simulation-Based Predictions of k_{off} Values: A Metadynamics Study. Journal of Physical Chemistry Letters, 2020, 11, 6373-6381.	4.6	41
22	Unified Approach to Enhanced Sampling. Physical Review X, 2020, 10, .	8.9	43
23	Tautomeric Equilibrium in Condensed Phases. Journal of Chemical Theory and Computation, 2020, 16, 6027-6031.	5.3	6
24	Integrating NMR and simulations reveals motions in the UUCG tetraloop. Nucleic Acids Research, 2020, 48, 5839-5848.	14.5	31
25	Path integral molecular dynamics for fermions: Alleviating the sign problem with the Bogoliubov inequality. Journal of Chemical Physics, 2020, 152, 171102.	3.0	23
26	Ab initio phase diagram and nucleation of gallium. Nature Communications, 2020, 11, 2654.	12.8	102
27	Molecular Mechanism of Gas Solubility in Liquid: Constant Chemical Potential Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5279-5286.	5.3	7
28	Gaussian Mixture-Based Enhanced Sampling for Statics and Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 5076-5080.	4.6	32
29	Rethinking Metadynamics: From Bias Potentials to Probability Distributions. Journal of Physical Chemistry Letters, 2020, 11, 2731-2736.	4.6	106
30	Variationally Enhanced Sampling. , 2020, , 621-634.		4
31	Data-Driven Collective Variables for Enhanced Sampling. Journal of Physical Chemistry Letters, 2020, 11, 2998-3004.	4.6	97
32	Metadynamics of Paths. Physical Review Letters, 2020, 125, 026001.	7.8	20
33	How Collective Phenomena Impact CO_2 Reactivity and Speciation in Different Media. Journal of Physical Chemistry A, 2020, 124, 3963-3975.	2.5	11
34	Kinetics of Aqueous Media Reactions via Ab Initio Enhanced Molecular Dynamics: The Case of Urea Decomposition. Journal of Physical Chemistry B, 2019, 123, 6851-6856.	2.6	9
35	Blind Search for Complex Chemical Pathways Using Harmonic Linear Discriminant Analysis. Journal of Chemical Theory and Computation, 2019, 15, 4507-4515.	5.3	19
36	Calculation of phase diagrams in the multithermal-multibaric ensemble. Journal of Chemical Physics, 2019, 150, 244119.	3.0	29

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37	Path integral molecular dynamics for bosons. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 21445-21449.	7.1	27
38	Molecular Dynamics Simulations of Crystal Nucleation from Solution at Constant Chemical Potential. Journal of Chemical Theory and Computation, 2019, 15, 6923-6930.	5.3	31
39	Neural networks-based variationally enhanced sampling. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 17641-17647.	7.1	90
40	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. Angewandte Chemie - International Edition, 2019, 58, 3976-3980.	13.8	23
41	Accurate Quantum Chemical Free Energies at Affordable Cost. Journal of Physical Chemistry Letters, 2019, 10, 3727-3731.	4.6	20
42	Temperature Dependence of Homogeneous Nucleation in Ice. Physical Review Letters, 2019, 122, 245501.	7.8	56
43	A local fingerprint for hydrophobicity and hydrophilicity: From methane to peptides. Journal of Chemical Physics, 2019, 150, 204103.	3.0	4
44	Exhaustive Search of Ligand Binding Pathways via Volume-Based Metadynamics. Journal of Physical Chemistry Letters, 2019, 10, 3495-3499.	4.6	59
45	Naphthalene crystal shape prediction from molecular dynamics simulations. CrystEngComm, 2019, 21, 3280-3288.	2.6	19
46	Making the Best of a Bad Situation: A Multiscale Approach to Free Energy Calculation. Journal of Chemical Theory and Computation, 2019, 15, 2187-2194.	5.3	18
47	Chasing the Full Free Energy Landscape of Neuroreceptor/Ligand Unbinding by Metadynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 3354-3361.	5.3	53
48	Improving collective variables: The case of crystallization. Journal of Chemical Physics, 2019, 150, 094509.	3.0	38
49	Multithermal-Multibaric Molecular Simulations from a Variational Principle. Physical Review Letters, 2019, 122, 050601.	7.8	22
50	Enhanced Sampling of Transition States. Journal of Chemical Theory and Computation, 2019, 15, 2454-2459.	5.3	16
51	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. Angewandte Chemie, 2019, 131, 4016-4020.	2.0	14
52	Microscopic description of acidâ€“base equilibrium. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4054-4057.	7.1	28
53	Enhanced Sampling of Protein Conformational Transitions via Dynamically Optimized Collective Variables. Journal of Chemical Theory and Computation, 2019, 15, 1393-1398.	5.3	18
54	Solvent-mediated morphology selection of the active pharmaceutical ingredient isoniazid: Experimental and simulation studies. Chemical Engineering Science, 2019, 204, 320-328.	3.8	35

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55	Accelerating the Calculation of Proteinâ€“Ligand Binding Free Energy and Residence Times Using Dynamically Optimized Collective Variables. Journal of Chemical Theory and Computation, 2019, 15, 743-750.	5.3	44
56	A Cannibalistic Approach to Grand Canonical Crystal Growth. Journal of Chemical Theory and Computation, 2018, 14, 2678-2683.	5.3	18
57	Searching for Entropically Stabilized Phases: The Case of Silver Iodide. Journal of Physical Chemistry C, 2018, 122, 1786-1790.	3.1	18
58	Refining Collective Coordinates and Improving Free Energy Representation in Variational Enhanced Sampling. Journal of Chemical Theory and Computation, 2018, 14, 2889-2894.	5.3	25
59	Folding a small protein using harmonic linear discriminant analysis. Journal of Chemical Physics, 2018, 149, 194113.	3.0	34
60	Silicon Liquid Structure and Crystal Nucleation from AbÂInitio Deep Metadynamics. Physical Review Letters, 2018, 121, 265701.	7.8	109
61	Variationally Enhanced Sampling. , 2018, , 1-14.		1
62	Quantum Symmetry from Enhanced Sampling Methods. Physical Review Letters, 2018, 121, 140602.	7.8	9
63	Combining Metadynamics and Integrated Tempering Sampling. Journal of Physical Chemistry Letters, 2018, 9, 6426-6430.	4.6	27
64	Metadynamics with Discriminants: A Tool for Understanding Chemistry. Journal of Chemical Theory and Computation, 2018, 14, 5040-5044.	5.3	45
65	Predicting polymorphism in molecular crystals using orientational entropy. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10251-10256.	7.1	57
66	Chemical potential calculations in non-homogeneous liquids. Journal of Chemical Physics, 2018, 149, 072305.	3.0	8
67	Frequency adaptive metadynamics for the calculation of rare-event kinetics. Journal of Chemical Physics, 2018, 149, 072309.	3.0	54
68	Molecular dynamics simulations of liquid silica crystallization. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5348-5352.	7.1	78
69	Collective Variables from Local Fluctuations. Journal of Physical Chemistry Letters, 2018, 9, 2776-2781.	4.6	101
70	Variational Flooding Study of a S_N2 Reaction. Journal of Physical Chemistry Letters, 2017, 8, 580-583.	4.6	23
71	Analyzing and Driving Cluster Formation in Atomistic Simulations. Journal of Chemical Theory and Computation, 2017, 13, 1317-1327.	5.3	82
72	Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E2136-E2145.	7.1	91

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73	1,3,5-tris(4-bromophenyl)-benzene Nucleation: From Dimers to Needle-like Clusters. Crystal Growth and Design, 2017, 17, 4137-4143.	3.0	9
74	Unbinding Kinetics of a p38 MAP Kinase Type II Inhibitor from Metadynamics Simulations. Journal of the American Chemical Society, 2017, 139, 4780-4788.	13.7	187
75	Coarse graining from variationally enhanced sampling applied to the Ginzburgâ€“Landau model. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3370-3374.	7.1	35
76	Concentration gradient driven molecular dynamics: a new method for simulations of membrane permeation and separation. Chemical Science, 2017, 8, 3858-3865.	7.4	66
77	Dimer Metadynamics. Journal of Chemical Theory and Computation, 2017, 13, 425-430.	5.3	8
78	Entropy based fingerprint for local crystalline order. Journal of Chemical Physics, 2017, 147, 114112.	3.0	92
79	Identifying Slow Molecular Motions in Complex Chemical Reactions. Journal of Physical Chemistry Letters, 2017, 8, 4197-4200.	4.6	12
80	Prion protein Î² 2â€“ Î± 2 loop conformational landscape. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9617-9622.	7.1	26
81	Conformational Entropy as Collective Variable for Proteins. Journal of Physical Chemistry Letters, 2017, 8, 4752-4756.	4.6	16
82	The impact of methylphenidate and its enantiomers on dopamine synthesis and metabolism in vitro. Progress in Neuro-Psychopharmacology and Biological Psychiatry, 2017, 79, 281-288.	4.8	12
83	Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations. Physical Review Letters, 2017, 119, 015701.	7.8	74
84	A variational conformational dynamics approach to the selection of collective variables in metadynamics. Journal of Chemical Physics, 2017, 147, 204109.	3.0	101
85	A variational approach to nucleation simulation. Faraday Discussions, 2016, 195, 557-568.	3.2	15
86	Application to large systems: general discussion. Faraday Discussions, 2016, 195, 671-698.	3.2	4
87	Communication: Role of explicit water models in the helix folding/unfolding processes. Journal of Chemical Physics, 2016, 145, 121101.	3.0	8
88	Overcoming time scale and finite size limitations to compute nucleation rates from small scale well tempered metadynamics simulations. Journal of Chemical Physics, 2016, 145, 211925.	3.0	40
89	Bespoke Bias for Obtaining Free Energy Differences within Variationally Enhanced Sampling. Journal of Chemical Theory and Computation, 2016, 12, 2162-2169.	5.3	11
90	Characterization of Vanadium Species in Mixed Chlorideâ€“Sulfate Solutions: An Ab Initio Metadynamics Study. Journal of Physical Chemistry C, 2016, 120, 10791-10798.	3.1	24

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91	Chemical potential calculations in dense liquids using metadynamics. European Physical Journal: Special Topics, 2016, 225, 1621-1628.	2.6	18
92	Hierarchical Protein Free Energy Landscapes from Variationally Enhanced Sampling. Journal of Chemical Theory and Computation, 2016, 12, 5751-5757.	5.3	5
93	Enhanced, targeted sampling of high-dimensional free-energy landscapes using variationally enhanced sampling, with an application to chignolin. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1150-1155.	7.1	47
94	General Protein Data Bank-Based Collective Variables for Protein Folding. Journal of Chemical Theory and Computation, 2016, 12, 29-35.	5.3	6
95	The interaction with gold suppresses fiber-like conformations of the amyloid Î² (16â€“22) peptide. Nanoscale, 2016, 8, 8737-8748.	5.6	55
96	Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint. Annual Review of Physical Chemistry, 2016, 67, 159-184.	10.8	497
97	Variationally Optimized Free-Energy Flooding for Rate Calculation. Physical Review Letters, 2015, 115, 070601.	7.8	35
98	A perturbative solution to metadynamics ordinary differential equation. Journal of Chemical Physics, 2015, 143, 234112.	3.0	13
99	Energetics and Structural Characterization of the large-scale Functional Motion of Adenylate Kinase. Scientific Reports, 2015, 5, 8425.	3.3	50
100	Molecular-dynamics simulations of urea nucleation from aqueous solution. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E6-14.	7.1	142
101	Probing the Unfolded Configurations of a Î²-Hairpin Using Sketch-Map. Journal of Chemical Theory and Computation, 2015, 11, 1086-1093.	5.3	25
102	Combustion Chemistry via Metadynamics: Benzyl Decomposition Revisited. Journal of Physical Chemistry A, 2015, 119, 978-989.	2.5	18
103	Path Integral Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 1383-1388.	5.3	21
104	Kinetics of proteinâ€“ligand unbinding: Predicting pathways, rates, and rate-limiting steps. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E386-91.	7.1	311
105	Heterogeneous Crystallization of the Phase Change Material GeTe via Atomistic Simulations. Journal of Physical Chemistry C, 2015, 119, 6428-6434.	3.1	28
106	Insight into the nucleation of urea crystals from the melt. Chemical Engineering Science, 2015, 121, 51-59.	3.8	70
107	Well-Tempered Variational Approach to Enhanced Sampling. Journal of Chemical Theory and Computation, 2015, 11, 1996-2002.	5.3	42
108	Urea homogeneous nucleation mechanism is solvent dependent. Faraday Discussions, 2015, 179, 291-307.	3.2	50

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109	Metadynamics studies of crystal nucleation. IUCrJ, 2015, 2, 256-266.	2.2	84
110	Molecular dynamics simulations of solutions at constant chemical potential. Journal of Chemical Physics, 2015, 142, 144113.	3.0	63
111	de Broglie Swapping Metadynamics for Quantum and Classical Sampling. Journal of Chemical Theory and Computation, 2015, 11, 5114-5119.	5.3	9
112	A Time-Independent Free Energy Estimator for Metadynamics. Journal of Physical Chemistry B, 2015, 119, 736-742.	2.6	399
113	G-triplex structure and formation propensity. Nucleic Acids Research, 2014, 42, 13393-13404.	14.5	71
114	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
115	Evaluating functions of positive-definite matrices using colored-noise thermostats. Physical Review E, 2014, 89, 023302.	2.1	4
116	Mechanistic insight into ligand binding to G-quadruplex DNA. Nucleic Acids Research, 2014, 42, 5447-5455.	14.5	79
117	Aqueous solutions: state of the art in ab initio molecular dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120482.	3.4	121
118	Anomalous water diffusion in salt solutions. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 3310-3315.	7.1	124
119	Well-Tempered Metadynamics Converges Asymptotically. Physical Review Letters, 2014, 112, 240602.	7.8	248
120	Assessing the Reliability of the Dynamics Reconstructed from Metadynamics. Journal of Chemical Theory and Computation, 2014, 10, 1420-1425.	5.3	175
121	Variational Approach to Enhanced Sampling and Free Energy Calculations. Physical Review Letters, 2014, 113, 090601.	7.8	206
122	Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-the-Fly Transition Barrier Estimation. Journal of Chemical Theory and Computation, 2014, 10, 3626-3633.	5.3	70
123	1,3,5-Tris(4-bromophenyl)benzene prenucleation clusters from metadynamics. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 132-136.	0.5	21
124	The role of the umbrella inversion mode in proton diffusion. Chemical Physics Letters, 2014, 599, 133-138.	2.6	31
125	Transient Polymorphism in NaCl. Journal of Chemical Theory and Computation, 2013, 9, 2526-2530.	5.3	44
126	Chiral, Racemic, and Meso-Lithium Tartrate Framework Polymorphs: A Detailed Structural Analysis. Crystal Growth and Design, 2013, 13, 3705-3715.	3.0	23

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127	Controlling and Predicting Crystal Shapes: The Case of Urea. Angewandte Chemie - International Edition, 2013, 52, 13369-13372.	13.8	89
128	Density functional simulations of hexagonal Ge2Sb2Te5at high pressure. Physical Review B, 2013, 87, .	3.2	5
129	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
130	From Metadynamics to Dynamics. Physical Review Letters, 2013, 111, 230602.	7.8	369
131	Proton transfer through the water gossamer. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13723-13728.	7.1	320
132	Water Release from Pyrophyllite during the Dehydroxylation Process Explored by Quantum Mechanical Simulations. Journal of Physical Chemistry C, 2013, 117, 7526-7532.	3.1	7
133	Funnel metadynamics as accurate binding free-energy method. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6358-6363.	7.1	337
134	The Gâ€Triplex DNA. Angewandte Chemie - International Edition, 2013, 52, 2269-2273.	13.8	133
135	Combining metadynamics simulation and experiments to characterize dendrimers in solution. Soft Matter, 2013, 9, 2593.	2.7	41
136	Demonstrating the Transferability and the Descriptive Power of Sketch-Map. Journal of Chemical Theory and Computation, 2013, 9, 1521-1532.	5.3	104
137	Thermodynamical Description of a Quasi-First-Order Phase Transition from the Well-Tempered Ensemble. Journal of Chemical Theory and Computation, 2013, 9, 5267-5276.	5.3	16
138	The allosteric communication pathways in KIX domain of CBP. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 14237-14242.	7.1	57
139	Free-energy landscape of protein oligomerization from atomistic simulations. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E4708-13.	7.1	79
140	Locating binding poses in protein-ligand systems using reconnaissance metadynamics. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5170-5175.	7.1	45
141	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
142	Sampling protein motion and solvent effect during ligand binding. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 1467-1472.	7.1	100
143	Uncovering Molecular Details of Urea Crystal Growth in the Presence of Additives. Journal of the American Chemical Society, 2012, 134, 17221-17233.	13.7	182
144	Counterion Redistribution upon Binding of a Tat-Protein Mimic to HIV-1 TAR RNA. Journal of Chemical Theory and Computation, 2012, 8, 688-694.	5.3	24

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145	Investigating the Mechanism of Substrate Uptake and Release in the Glutamate Transporter Homologue Glt_{Ph} through Metadynamics Simulations. Journal of the American Chemical Society, 2012, 134, 453-463.	13.7	66
146	Combined Computational and Experimental NMR Study of Calix[4]arene Derivatives. Journal of Physical Chemistry C, 2012, 116, 23441-23452.	3.1	1
147	Metadynamics with Adaptive Gaussians. Journal of Chemical Theory and Computation, 2012, 8, 2247-2254.	5.3	220
148	The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates. Journal of the American Chemical Society, 2012, 134, 8557-8569.	13.7	45
149	Microscopic Origins of the Anomalous Melting Behavior of Sodium under High Pressure. Physical Review Letters, 2012, 108, 115701.	7.8	64
150	Accelerating the convergence of path integral dynamics with a generalized Langevin equation. Journal of Chemical Physics, 2011, 134, 084104.	3.0	139
151	Static disorder and structural correlations in the low-temperature phase of lithium imide. Physical Review B, 2011, 83, .	3.2	12
152	Structural Diversity and Energetics in Anhydrous Lithium Tartrates: Experimental and Computational Studies of Novel Chiral Polymorphs and Their Racemic and Meso Analogues. Crystal Growth and Design, 2011, 11, 221-230.	3.0	39
153	First-Principles Study of the High-Temperature Phase of Li₂NH. Journal of Physical Chemistry C, 2011, 115, 7076-7080.	3.1	7
154	Hydrogen Oxidation Reaction at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ni</mml:mi><mml:mo>/</mml:mo><mml:mi>YSZ</mml:mi></mml:math>Anode of Solid Oxide Fuel Cells from First Principles. Physical Review Letters, 2011, 107, 206103.	7.8	38
155	Replica Temperatures for Uniform Exchange and Efficient Roundtrip Times in Explicit Solvent Parallel Tempering Simulations. Journal of Chemical Theory and Computation, 2011, 7, 2025-2027.	5.3	63
156	Effect of Urea on the Î²-Hairpin Conformational Ensemble and Protein Denaturation Mechanism. Journal of the American Chemical Society, 2011, 133, 17200-17206.	13.7	59
157	On the recombination of hydronium and hydroxide ions in water. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 20410-20415.	7.1	154
158	Nucleation mechanism for the direct graphite-to-diamond phase transition. Nature Materials, 2011, 10, 693-697.	27.5	277
159	Metadynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 826-843.	14.6	971
160	A chiralityâ€based metrics for freeâ€energy calculations in biomolecular systems. Journal of Computational Chemistry, 2011, 32, 2627-2637.	3.3	25
161	Intramolecular Weak Interactions in the Thermodynamic Stereoselectivity of Copper(II) Complexes with Carnosineâ€“Trehalose Conjugates. Chemistry - A European Journal, 2011, 17, 9448-9455.	3.3	24
162	Exploring the free energy surfaces of clusters using reconnaissance metadynamics. Journal of Chemical Physics, 2011, 135, 114109.	3.0	20

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163	Momentum distribution, vibrational dynamics, and the potential of mean force in ice. Physical Review B, 2011, 83, .	3.2	33
164	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
165	Targeting biomolecular flexibility with metadynamics. Current Opinion in Structural Biology, 2010, 20, 148-154.	5.7	127
166	Multiple Routes and Milestones in the Folding of HIVâ€“1 Protease Monomer. PLoS ONE, 2010, 5, e13208.	2.5	15
167	Displaced Path Integral Formulation for the Momentum Distribution of Quantum Particles. Physical Review Letters, 2010, 105, 110602.	7.8	49
168	First-principles study of liquid and amorphous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Sb</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2010, 81, .	3.2	94
169	Nuclear quantum effects inab initiodynamics: Theory and experiments for lithium imide. Physical Review B, 2010, 82, .	3.2	43
170	Molecular basis of cyclooxygenase enzymes (COXs) selective inhibition. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5411-5416.	7.1	187
171	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
172	Signature of Tetrahedral Ge in the Raman Spectrum of Amorphous Phase-Change Materials. Physical Review Letters, 2010, 104, 085503.	7.8	164
173	Asprich Peptides Are Occluded in Calcite and Permanently Disorder Biomineral Crystals. Journal of the American Chemical Society, 2010, 132, 11585-11591.	13.7	68
174	Colored-Noise Thermostats Ã la Carte. Journal of Chemical Theory and Computation, 2010, 6, 1170-1180.	5.3	199
175	Linking Well-Tempered Metadynamics Simulations with Experiments. Biophysical Journal, 2010, 98, L44-L46.	0.5	56
176	Probing the Mechanism of pH-Induced Large-Scale Conformational Changes in Dengue Virus Envelope Protein Using Atomistic Simulations. Biophysical Journal, 2010, 99, 588-594.	0.5	33
177	Efficient stochastic thermostatting of path integral molecular dynamics. Journal of Chemical Physics, 2010, 133, 124104.	3.0	259
178	Ab initioquality neural-network potential for sodium. Physical Review B, 2010, 81, .	3.2	115
179	Enhanced Sampling in the Well-Tempered Ensemble. Physical Review Letters, 2010, 104, 190601.	7.8	225
180	Graphite-diamond phase coexistence study employing a neural-network mapping of theab initiopotential energy surface. Physical Review B, 2010, 81, .	3.2	100

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181	First Principles Study of the LiNH₂/Li₂NH Transformation. Journal of Physical Chemistry C, 2010, 114, 15174-15183.	3.1	33
182	A Hybrid Approach to Fermi Operator Expansion. , 2009, , .		11
183	Superionic Conduction in Substoichiometric LiAl Alloy: AnAbÂInitioStudy. Physical Review Letters, 2009, 103, 125901.	7.8	21
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