Michele Parrinello

List of Publications by Year
in descending order

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	Polymorphic transitions in single crystals: A new molecular dynamics method. Journal of Applied Physics, 1981, 52, 7182-7190.	2.5	14,777
2	Canonical sampling through velocity rescaling. Journal of Chemical Physics, 2007, 126, 014101.	3.0	11,867
3	Unified Approach for Molecular Dynamics and Density-Functional Theory. Physical Review Letters, 1985, 55, 2471-2474.	7.8	9,715
4	Escaping free-energy minima. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12562-12566.	7.1	4,527
5	Quickstep: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach. Computer Physics Communications, 2005, 167, 103-128.	7.5	4,200
6	Crystal Structure and Pair Potentials: A Molecular-Dynamics Study. Physical Review Letters, 1980, 45, 1196-1199.	7.8	2,873
7	Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces. Physical Review Letters, 2007, 98, 146401.	7.8	2,677
8	Well-Tempered Metadynamics: A Smoothly Converging and Tunable Free-Energy Method. Physical Review Letters, 2008, 100, 020603.	7.8	2,201
9	The nature of the hydrated excess proton in water. Nature, 1999, 397, 601-604.	27.8	1,587
10	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. Computer Physics Communications, 2009, 180, 1961-1972.	7.5	1,448
11	Metadynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 826-843.	14.6	971
12	A hybrid Gaussian and plane wave density functional scheme. Molecular Physics, 1997, 92, 477-487.	1.7	881
13	The nature and transport mechanism of hydrated hydroxide ions in aqueous solution. Nature, 2002, 417, 925-929.	27.8	858
14	Efficient Exploration of Reactive Potential Energy Surfaces Using Car-Parrinello Molecular Dynamics. Physical Review Letters, 2003, 90, 238302.	7.8	719
15	On the Quantum Nature of the Shared Proton in Hydrogen Bonds. Science, 1997, 275, 817-820.	12.6	679
16	Autoionization in Liquid Water. Science, 2001, 291, 2121-2124.	12.6	672
17	Ab initio molecular dynamics simulation of liquid water: Comparison of three gradientâ€corrected density functionals. Journal of Chemical Physics, 1996, 105, 1142-1152.	3.0	597
18	Study of an F center in molten KCl. Journal of Chemical Physics, 1984, 80, 860-867.	3.0	580

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19	Water Molecule Dipole in the Gas and in the Liquid Phase. Physical Review Letters, 1999, 82, 3308-3311.	7.8	563
20	Structural, electronic, and bonding properties of liquid water from first principles. Journal of Chemical Physics, 1999, 111, 3572-3580.	3.0	547
21	Ab Initio Molecular Dynamics Simulation of the Solvation and Transport of H3O+ and OH- Ions in Water. The Journal of Physical Chemistry, 1995, 99, 5749-5752.	2.9	545
22	The Gaussian and augmented-plane-wave density functional method for ab initio molecular dynamics simulations. Theoretical Chemistry Accounts, 1999, 103, 124-140.	1.4	513
23	Efficient Reconstruction of Complex Free Energy Landscapes by Multiple Walkers Metadynamicsâ€. Journal of Physical Chemistry B, 2006, 110, 3533-3539.	2.6	511
24	Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint. Annual Review of Physical Chemistry, 2016, 67, 159-184.	10.8	497
25	From A to B in free energy space. Journal of Chemical Physics, 2007, 126, 054103.	3.0	476
26	Free-Energy Landscape for Î² Hairpin Folding from Combined Parallel Tempering and Metadynamics. Journal of the American Chemical Society, 2006, 128, 13435-13441.	13.7	458
27	Assessing the Accuracy of Metadynamicsâ€. Journal of Physical Chemistry B, 2005, 109, 6714-6721.	2.6	446
28	The influence of temperature and density functional models in ab initio molecular dynamics simulation of liquid water. Journal of Chemical Physics, 2005, 122, 014515.	3.0	444
29	Ab initio path integral molecular dynamics: Basic ideas. Journal of Chemical Physics, 1996, 104, 4077-4082.	3.0	414
30	A Time-Independent Free Energy Estimator for Metadynamics. Journal of Physical Chemistry B, 2015, 119, 736-742.	2.6	399
31	Tunnelling and zero-point motion in high-pressure ice. Nature, 1998, 392, 258-261.	27.8	389
32	Effective force fields for condensed phase systems from ab initio molecular dynamics simulation: A new method for force-matching. Journal of Chemical Physics, 2004, 120, 10896-10913.	3.0	383
33	Structural, Dymanical, and Electronic Properties of Amorphous Silicon: Anab initioMolecular-Dynamics Study. Physical Review Letters, 1988, 60, 204-207.	7.8	369
34	From Metadynamics to Dynamics. Physical Review Letters, 2013, 111, 230602.	7.8	369
35	Maximally-localized Wannier functions for disordered systems: Application to amorphous silicon. Solid State Communications, 1998, 107, 7-11.	1.9	363
36	Equilibrium Geometries and Electronic Structure of Ironâ€'Porphyrin Complexes:â€‰ A Density Functional Study. Journal of Physical Chemistry A, 1997, 101, 8914-8925.	2.5	362

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37	Equilibrium Free Energies from Nonequilibrium Metadynamics. Physical Review Letters, 2006, 96, 090601.	7.8	355
38	Efficient and Accurate Car-Parrinello-like Approach to Born-Oppenheimer Molecular Dynamics. Physical Review Letters, 2007, 98, 066401.	7.8	351
39	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
40	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	2.6	327
41	Ab initio infrared spectrum of liquid water. Chemical Physics Letters, 1997, 277, 478-482.	2.6	325
42	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
43	Large scale electronic structure calculations. Physical Review Letters, 1992, 69, 3547-3550.	7.8	317
44	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
45	Efficient and general algorithms for path integral Carâ€“Parrinello molecular dynamics. Journal of Chemical Physics, 1996, 104, 5579-5588.	3.0	303
46	Structural and Electronic Properties of Amorphous Carbon. Physical Review Letters, 1989, 62, 555-558.	7.8	301
47	Isothermal-isobaric molecular dynamics using stochastic velocity rescaling. Journal of Chemical Physics, 2009, 130, 074101.	3.0	297
48	Reconstructing the equilibrium Boltzmann distribution from wellâ€tempered metadynamics. Journal of Computational Chemistry, 2009, 30, 1615-1621.	3.3	297
49	The Role and Perspective of Ab Initio Molecular Dynamics in the Study of Biological Systems. Accounts of Chemical Research, 2002, 35, 455-464.	15.6	287
50	Hydrogen Bonding in Water. Physical Review Letters, 2003, 91, 215503.	7.8	284
51	Dispersion corrections to density functionals for water aromatic interactions. Journal of Chemical Physics, 2004, 120, 2693-2699.	3.0	283
52	Equilibrium Structures and Finite Temperature Properties of Silicon Microclusters fromab initioMolecular-Dynamics Calculations. Physical Review Letters, 1988, 60, 271-274.	7.8	279
53	Nucleation mechanism for the direct graphite-to-diamond phase transition. Nature Materials, 2011, 10, 693-697.	27.5	277
54	General and efficient algorithms for obtaining maximally localized Wannier functions. Physical Review B, 2000, 61, 10040-10048.	3.2	272

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55	Flexible Docking in Solution Using Metadynamics. Journal of the American Chemical Society, 2005, 127, 2600-2607.	13.7	266
56	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
57	Efficient stochastic thermostatting of path integral molecular dynamics. Journal of Chemical Physics, 2010, 133, 124104.	3.0	259
58	Ab initiocalculation of properties of carbon in the amorphous and liquid states. Physical Review B, 1990, 42, 7470-7482.	3.2	258
59	Accurate sampling using Langevin dynamics. Physical Review E, 2007, 75, 056707.	2.1	257
60	Molecular dynamics in low-spin excited states. Journal of Chemical Physics, 1998, 108, 4060-4069.	3.0	249
61	Well-Tempered Metadynamics Converges Asymptotically. Physical Review Letters, 2014, 112, 240602.	7.8	248
62	A Recipe for the Computation of the Free Energy Barrier and the Lowest Free Energy Path of Concerted Reactionsâ€. Journal of Physical Chemistry B, 2005, 109, 6676-6687.	2.6	243
63	First Principles Molecular Dynamics Study of Zieglerâ^'Natta Heterogeneous Catalysis. Journal of the American Chemical Society, 1998, 120, 2746-2752.	13.7	229
64	Ab InitioMolecular Dynamics with Excited Electrons. Physical Review Letters, 1994, 73, 2599-2602.	7.8	227
65	Freezing of a Lennard-Jones Fluid: From Nucleation to Spinodal Regime. Physical Review Letters, 2006, 97, 105701.	7.8	227
66	Enhanced Sampling in the Well-Tempered Ensemble. Physical Review Letters, 2010, 104, 190601.	7.8	225
67	An Efficient Real Space Multigrid QM/MM Electrostatic Coupling. Journal of Chemical Theory and Computation, 2005, 1, 1176-1184.	5.3	224
68	Metadynamics with Adaptive Gaussians. Journal of Chemical Theory and Computation, 2012, 8, 2247-2254.	5.3	220
69	Anisotropy of Earth's Dâ€³ layer and stacking faults in the MgSiO3 post-perovskite phase. Nature, 2005, 438, 1142-1144.	27.8	219
70	Ab initio path-integral molecular dynamics. European Physical Journal B, 1994, 95, 143-144.	1.5	216
71	Ab initioMolecular Dynamics Simulation of Laser Melting of Silicon. Physical Review Letters, 1996, 77, 3149-3152.	7.8	216
72	A New ab-Initio Approach for NMR Chemical Shifts in Periodic Systems. Journal of Physical Chemistry A, 2001, 105, 1951-1958.	2.5	207

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73	Metadynamics Simulations of the High-Pressure Phases of Silicon Employing a High-Dimensional Neural Network Potential. Physical Review Letters, 2008, 100, 185501.	7.8	207
74	Variational Approach to Enhanced Sampling and Free Energy Calculations. Physical Review Letters, 2014, 113, 090601.	7.8	206
75	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
76	Colored-Noise Thermostats Ã la Carte. Journal of Chemical Theory and Computation, 2010, 6, 1170-1180.	5.3	199
77	First Principles Study of Propene Polymerization in Zieglerâ^'Natta Heterogeneous Catalysis. Journal of the American Chemical Society, 2000, 122, 501-509.	13.7	198
78	Crystal structure transformations in SiO2 from classical and ab initio metadynamics. Nature Materials, 2006, 5, 623-626.	27.5	198
79	The Conformational Free Energy Landscape of Î²-<scp>d</scp>-Glucopyranose. Implications for Substrate Preactivation in Î²-Glucoside Hydrolases. Journal of the American Chemical Society, 2007, 129, 10686-10693.	13.7	196
80	Structural quantum effects and three-centre two-electron bonding in CH+5. Nature, 1995, 375, 216-218.	27.8	190
81	Water structure as a function of temperature from X-ray scattering experiments and ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2003, 5, 1981.	2.8	189
82	Static and Dynamical Properties of Liquid Water from First Principles by a Novel Carâ^'Parrinello-like Approach. Journal of Chemical Theory and Computation, 2009, 5, 235-241.	5.3	189
83	Nuclear Quantum Effects in Solids Using a Colored-Noise Thermostat. Physical Review Letters, 2009, 103, 030603.	7.8	188
84	All-electron ab-initio molecular dynamics. Physical Chemistry Chemical Physics, 2000, 2, 2105-2112.	2.8	187
85	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
86	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
87	Generalized variational density functional perturbation theory. Journal of Chemical Physics, 2000, 113, 7102-7109.	3.0	183
88	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
89	Ab initiomolecular-dynamics simulation of K+ solvation in water. Journal of Chemical Physics, 1999, 111, 1587-1591.	3.0	178
90	Integrating the Carâ€"Parrinello equations. I. Basic integration techniques. Journal of Chemical Physics, 1994, 101, 1302-1315.	3.0	175

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91	Assessing the Reliability of the Dynamics Reconstructed from Metadynamics. Journal of Chemical Theory and Computation, 2014, 10, 1420-1425.	5.3	175
92	Impurity states in doped fullerenes: C59B and C59N. Chemical Physics Letters, 1992, 190, 159-162.	2.6	171
93	From silicon to RNA: The coming of age of ab initio molecular dynamics. Solid State Communications, 1997, 102, 107-120.	1.9	171
94	Hydrolysis at stepped MgO surfaces. Physical Review Letters, 1994, 73, 504-507.	7.8	170
95	Langevin Equation with Colored Noise for Constant-Temperature Molecular Dynamics Simulations. Physical Review Letters, 2009, 102, 020601.	7.8	170
96	Pulling Monatomic Gold Wires with Single Molecules: AnAb InitioSimulation. Physical Review Letters, 2002, 89, 186402.	7.8	169
97	Signature of Tetrahedral Ge in the Raman Spectrum of Amorphous Phase-Change Materials. Physical Review Letters, 2010, 104, 085503.	7.8	164
98	Ab initio molecular dynamics of ion solvation. The case of Be2+ in water. Chemical Physics Letters, 1997, 273, 360-366.	2.6	159
99	Electronic Structure of Wet DNA. Physical Review Letters, 2002, 89, 108102.	7.8	157
100	First-Principles Molecular-Dynamics Simulations of a Hydrated Electron in Normal and Supercritical Water. Physical Review Letters, 2003, 90, 226403.	7.8	156
101	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
102	An Efficient Linear-Scaling Electrostatic Coupling for Treating Periodic Boundary Conditions in QM/MM Simulations. Journal of Chemical Theory and Computation, 2006, 2, 1370-1378.	5.3	152
103	Î±-gallium: A metallic molecular crystal. Physical Review B, 1991, 43, 14277-14280.	3.2	151
104	Hydrogen Bonding and Dipole Moment of Water at Supercritical Conditions: A First-Principles Molecular Dynamics Study. Physical Review Letters, 2000, 85, 3245-3248.	7.8	151
105	Energy Conservation in Adaptive Hybrid Atomistic/Coarse-Grain Molecular Dynamics. Journal of Chemical Theory and Computation, 2007, 3, 1100-1105.	5.3	151
106	Reconstructing the Density of States by History-Dependent Metadynamics. Physical Review Letters, 2004, 92, 170601.	7.8	149
107	Surface solvation of halogen anions in water clusters: An ab initio molecular dynamics study of the Clâ^'(H2O)6 complex. Journal of Chemical Physics, 2001, 114, 7036-7044.	3.0	148
108	Electronic structure optimization in plane-wave-based density functional calculations by direct inversion in the iterative subspace. Computational Materials Science, 1994, 2, 244-248.	3.0	147

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109	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
110	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
111	Accelerating the convergence of path integral dynamics with a generalized Langevin equation. Journal of Chemical Physics, 2011, 134, 084104.	3.0	139
112	Exploring Polymorphism: The Case of Benzene. Angewandte Chemie - International Edition, 2005, 44, 3769-3773.	13.8	138
113	Interaction of short-chain alkane thiols and thiolates with small gold clusters: Adsorption structures and energetics. Journal of Chemical Physics, 2001, 115, 4776-4786.	3.0	136
114	Action-Derived Molecular Dynamics in the Study of Rare Events. Physical Review Letters, 2001, 87, 108302.	7.8	134
115	The Gâ€Triplex DNA. Angewandte Chemie - International Edition, 2013, 52, 2269-2273.	13.8	133
116	Microscopic struture of amorphous covalent alloys probed byab initiomolecular dynamics: SiC. Physical Review Letters, 1992, 68, 3044-3047.	7.8	132
117	Role of Conformational Fluctuations in the Enzymatic Reaction of HIV-1 Protease. Journal of Molecular Biology, 2002, 319, 567-583.	4.2	130
118	Protein Conformational Transitions: The Closure Mechanism of a Kinase Explored by Atomistic Simulations. Journal of the American Chemical Society, 2009, 131, 244-250.	13.7	130
119	Influence of the Heme Pocket Conformation on the Structure and Vibrations of the Fe-CO Bond in Myoglobin: A QM/MM Density Functional Study. Biophysical Journal, 2001, 81, 435-445.	0.5	128
120	Targeting biomolecular flexibility with metadynamics. Current Opinion in Structural Biology, 2010, 20, 148-154.	5.7	127
121	Hydrogen Bond Driven Chemical Reactions:Â Beckmann Rearrangement of Cyclohexanone Oxime into Îµ-Caprolactam in Supercritical Water. Journal of the American Chemical Society, 2004, 126, 6280-6286.	13.7	125
122	Ab Initio Molecular Dynamics-Based Assignment of the Protonation State of Pepstatin A/HIV-1 Protease Cleavage Site. Journal of the American Chemical Society, 2001, 123, 8730-8737.	13.7	124
123	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
124	A First Principles Exploration of a Variety of Active Surfaces and Catalytic Sites in Zieglerâ^'Natta Heterogeneous Catalysis. Journal of Physical Chemistry A, 2001, 105, 5096-5105.	2.5	123
125	Water at supercritical conditions: A first principles study. Journal of Chemical Physics, 2001, 115, 2219-2227.	3.0	123
126	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

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127	Electronic and vibrational properties ofC60at finite temperature fromab initiomolecular dynamics. Physical Review B, 1991, 44, 4056-4059.	3.2	119
128	Anharmonic Raman Spectra in High-Pressure Ice fromAb InitioSimulations. Physical Review Letters, 2002, 88, 176401.	7.8	119
129	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
130	A Molecular Dynamics Study of the Early Stages of Calcium Carbonate Growth. Journal of Physical Chemistry B, 2009, 113, 11680-11687.	2.6	116
131	Ab initioquality neural-network potential for sodium. Physical Review B, 2010, 81, .	3.2	115
132	Carbon: The nature of the liquid state. Physical Review Letters, 1989, 63, 988-991.	7.8	113
133	Reconstruction of the diamond (111) surface. Physical Review Letters, 1992, 69, 2947-2950.	7.8	113
134	Ab-Initio Molecular Dynamics: Principles and Practical Implementation. , 1991, , 283-304.		112
135	Stochastic thermostats: comparison of local and global schemes. Computer Physics Communications, 2008, 179, 26-29.	7.5	112
136	Silicon Liquid Structure and Crystal Nucleation from AbÂInitio Deep Metadynamics. Physical Review Letters, 2018, 121, 265701.	7.8	109
137	Medium Effects on51V NMR Chemical Shifts: A Density Functional Study. Chemistry - A European Journal, 2001, 7, 4487-4494.	3.3	108
138	Ab initiosimulation of water interaction with the (100) surface of pyrite. Journal of Chemical Physics, 2003, 118, 8917-8926.	3.0	108
139	Nucleotide-dependent conformational states of actin. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 12723-12728.	7.1	106
140	Rethinking Metadynamics: From Bias Potentials to Probability Distributions. Journal of Physical Chemistry Letters, 2020, 11, 2731-2736.	4.6	106
141	Solvation Structure and Mobility Mechanism of OH-:â€‰ A Carâ€™Parrinello Molecular Dynamics Investigation of Alkaline Solutions. Journal of Physical Chemistry B, 2002, 106, 12006-12016.	2.6	105
142	Metadynamics Simulation of Prion Protein:Â Î²-Structure Stability and the Early Stages of Misfolding. Journal of the American Chemical Society, 2006, 128, 2705-2710.	13.7	105
143	Demonstrating the Transferability and the Descriptive Power of Sketch-Map. Journal of Chemical Theory and Computation, 2013, 9, 1521-1532.	5.3	104
144	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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145	A possible new highly stable fulleride cluster: Li12C60. Chemical Physics Letters, 1992, 198, 472-477.	2.6	102
146	Stability and Structure of Oligomers of the Alzheimer Peptide AÎ²16â€“22: From the Dimer to the 32-Mer. Biophysical Journal, 2006, 91, 3217-3229.	0.5	102
147	Ab initio phase diagram and nucleation of gallium. Nature Communications, 2020, 11, 2654.	12.8	102
148	A variational conformational dynamics approach to the selection of collective variables in metadynamics. Journal of Chemical Physics, 2017, 147, 204109.	3.0	101
149	Collective Variables from Local Fluctuations. Journal of Physical Chemistry Letters, 2018, 9, 2776-2781.	4.6	101
150	Dissociation Mechanism of Acetic Acid in Water. Journal of the American Chemical Society, 2006, 128, 11318-11319.	13.7	100
151	Graphite-diamond phase coexistence study employing a neural-network mapping of theab initiopotential energy surface. Physical Review B, 2010, 81, .	3.2	100
152	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
153	Density Functional Theory-Based Molecular Dynamics Simulation of Acid-Catalyzed Chemical Reactions in Liquid Trioxane. Journal of the American Chemical Society, 1997, 119, 7218-7229.	13.7	97
154	The Unfolded Ensemble and Folding Mechanism of the C-Terminal GB1 Î²-Hairpin. Journal of the American Chemical Society, 2008, 130, 13938-13944.	13.7	97
155	Data-Driven Collective Variables for Enhanced Sampling. Journal of Physical Chemistry Letters, 2020, 11, 2998-3004.	4.6	97
156	Ab initio molecular dynamics simulation of liquid hydrogen fluoride. Journal of Chemical Physics, 1997, 106, 4658-4664.	3.0	95
157	Integrating the Carâ€“Parrinello equations. II. Multiple time scale techniques. Journal of Chemical Physics, 1994, 101, 1316-1329.	3.0	94
158	The Role of the Peripheral Anionic Site and Cationâ^Ï€ Interactions in the Ligand Penetration of the Human AChE Gorge. Journal of the American Chemical Society, 2005, 127, 9147-9155.	13.7	94
159	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
160	Microscopic Mechanism of Antibiotics Translocation through a Porin. Biophysical Journal, 2004, 87, 58-64.	0.5	92
161	Simulation of structural phase transitions by metadynamics. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	92
162	Entropy based fingerprint for local crystalline order. Journal of Chemical Physics, 2017, 147, 114112.	3.0	92

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163	Structure and bonding in cisplatin and other Pt(II) complexes. Chemical Physics Letters, 1995, 234, 50-56.	2.6	91
164	MOLECULAR SPECTROSCOPY:CH5+: The Cheshire Cat Smiles. Science, 1999, 284, 59-61.	12.6	91
165	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
166	Structural, dynamical, electronic, and bonding properties of laser-heated silicon: Anab initiomolecular-dynamics study. Physical Review B, 1997, 56, 3806-3812.	3.2	90
167	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
168	Confinement effects and acid strength in zeolites. Nature Communications, 2021, 12, 2630.	12.8	90
169	Controlling and Predicting Crystal Shapes: The Case of Urea. Angewandte Chemie - International Edition, 2013, 52, 13369-13372.	13.8	89
170	Understanding the Nature of Water Bound to Solid Acid Surfaces. Ab Initio Simulation on HSAPO-34. Journal of the American Chemical Society, 1998, 120, 8512-8516.	13.7	87
171	Solvated excess protons in water: quantum effects on the hydration structure. Journal of Physics Condensed Matter, 2000, 12, A153-A159.	1.8	86
172	First-Principles Study of Aqueous Hydroxide Solutions. Journal of the American Chemical Society, 2002, 124, 8534-8535.	13.7	86
173	The dissociation mechanism of H2O in water studied by first-principles molecular dynamics. Chemical Physics Letters, 1998, 288, 343-347.	2.6	85
174	Structural and electronic properties of C70. Chemical Physics Letters, 1992, 189, 241-244.	2.6	84
175	Structural and Electronic Properties of Co-corrole, Co-corrin, and Co-porphyrin. Inorganic Chemistry, 2001, 40, 11-17.	4.0	84
176	Metadynamics studies of crystal nucleation. IUCrJ, 2015, 2, 256-266.	2.2	84
177	At the Water's Edge:â€‰ Nitric Acid as a Weak Acid. Journal of the American Chemical Society, 2007, 129, 12910-12911.	13.7	82
178	Analyzing and Driving Cluster Formation in Atomistic Simulations. Journal of Chemical Theory and Computation, 2017, 13, 1317-1327.	5.3	82
179	Density-functional study of hydration of sodium in water clusters. Journal of Chemical Physics, 1998, 109, 6839-6843.	3.0	80
180	Ab Initio Simulation of Rotational Dynamics of Solvated Ammonium Ion in Water. Journal of the American Chemical Society, 1999, 121, 10883-10888.	13.7	79

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181	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
182	Mechanistic insight into ligand binding to G-quadruplex DNA. Nucleic Acids Research, 2014, 42, 5447-5455.	14.5	79
183	Analysis of the Dissociation of H2O in Water Using First-Principles Molecular Dynamics. Journal of Physical Chemistry B, 1999, 103, 7340-7345.	2.6	78
184	Azulene-to-Naphthalene Rearrangement: The Car-Parrinello Metadynamics Method Explores Various Reaction Mechanisms. ChemPhysChem, 2004, 5, 1558-1568.	2.1	78
185	Phase Selection and Energetics in Chiral Alkaline Earth Tartrates and Their Racemic and Meso Analogues: Synthetic, Structural, Computational, and Calorimetric Studies. Journal of the American Chemical Society, 2009, 131, 15375-15386.	13.7	78
186	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
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