Weitao Yang

List of Publications by Year
in descending order

361 papers	134,720 citations	3731 89 h-index	663 255 g-index
365 all docs	365 docs citations	365 times ranked	72814 citing authors

#	Article	IF	Citations
1	Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. Physical Review B, 1988, 37, 785-789.	3.2	86,607
2	Revealing Noncovalent Interactions. Journal of the American Chemical Society, 2010, 132, 6498-6506.	13.7	6,465
3	Density functional approach to the frontier-electron theory of chemical reactivity. Journal of the American Chemical Society, 1984, 106, 4049-4050.	13.7	2,940
4	NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	5.3	2,897
5	Comment on â€œGeneralized Gradient Approximation Made Simpleâ€. Physical Review Letters, 1998, 80, 890-890.	7.8	2,323
6	Insights into Current Limitations of Density Functional Theory. Science, 2008, 321, 792-794.	12.6	2,057
7	Challenges for Density Functional Theory. Chemical Reviews, 2012, 112, 289-320.	47.7	1,869
8	The use of global and local molecular parameters for the analysis of the gas-phase basicity of amines. Journal of the American Chemical Society, 1986, 108, 5708-5711.	13.7	1,598
9	Hardness, softness, and the fukui function in the electronic theory of metals and catalysis.. Proceedings of the National Academy of Sciences of the United States of America, 1985, 82, 6723-6726.	7.1	1,436
10	Localization and Delocalization Errors in Density Functional Theory and Implications for Band-Gap Prediction. Physical Review Letters, 2008, 100, 146401.	7.8	1,012
11	Direct calculation of electron density in density-functional theory. Physical Review Letters, 1991, 66, 1438-1441.	7.8	943
12	Density-Functional Theory of the Electronic Structure of Molecules. Annual Review of Physical Chemistry, 1995, 46, 701-728.	10.8	903
13	Empirical correction to density functional theory for van der Waals interactions. Journal of Chemical Physics, 2002, 116, 515-524.	3.0	762
14	Layer-Dependent Electrocatalysis of MoS₂ for Hydrogen Evolution. Nano Letters, 2014, 14, 553-558.	9.1	667
15	All The Catalytic Active Sites of MoS₂ for Hydrogen Evolution. Journal of the American Chemical Society, 2016, 138, 16632-16638.	13.7	664
16	Many-electron self-interaction error in approximate density functionals. Journal of Chemical Physics, 2006, 125, 201102.	3.0	630
17	A challenge for density functionals: Self-interaction error increases for systems with a noninteger number of electrons. Journal of Chemical Physics, 1998, 109, 2604-2608.	3.0	524
18	A densityâ€matrix divideâ€andâ€conquer approach for electronic structure calculations of large molecules. Journal of Chemical Physics, 1995, 103, 5674-5678.	3.0	499

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19	Fractional charge perspective on the band gap in density-functional theory. Physical Review B, 2008, 77, .	3.2	491
20	A pseudobond approach to combining quantum mechanical and molecular mechanical methods. Journal of Chemical Physics, 1999, 110, 46-54.	3.0	460
21	Electron density, Kohnâ€“Sham frontier orbitals, and Fukui functions. Journal of Chemical Physics, 1984, 81, 2862-2863.	3.0	441
22	Free energy calculation on enzyme reactions with an efficient iterative procedure to determine minimum energy paths on a combinedab initioQM/MM potential energy surface. Journal of Chemical Physics, 2000, 112, 3483-3492.	3.0	434
23	Understanding band gaps of solids in generalized Kohnâ€“Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
24	Free Energies of Chemical Reactions in Solution and in Enzymes with Ab Initio Quantum Mechanics/Molecular Mechanics Methods. Annual Review of Physical Chemistry, 2008, 59, 573-601.	10.8	394
25	Degenerate Ground States and a Fractional Number of Electrons in Density and Reduced Density Matrix Functional Theory. Physical Review Letters, 2000, 84, 5172-5175.	7.8	390
26	Product selectivity in plasmonic photocatalysis for carbon dioxide hydrogenation. Nature Communications, 2017, 8, 14542.	12.8	348
27	Analysis of Hydrogen-Bond Interaction Potentials from the Electron Density: Integration of Noncovalent Interaction Regions. Journal of Physical Chemistry A, 2011, 115, 12983-12990.	2.5	339
28	Concerted O atomâ€“proton transfer in the Oâ€”O bond forming step in water oxidation. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 7225-7229.	7.1	295
29	Development of exchange-correlation functionals with minimal many-electron self-interaction error. Journal of Chemical Physics, 2007, 126, 191109.	3.0	290
30	Describing van der Waals Interaction in diatomic molecules with generalized gradient approximations: The role of the exchange functional. Journal of Chemical Physics, 1997, 107, 7921-7925.	3.0	282
31	A direct optimization method for calculating density functionals and exchangeâ€“correlation potentials from electron densities. Journal of Chemical Physics, 2003, 118, 2498.	3.0	267
32	Plasmon-Enhanced Catalysis: Distinguishing Thermal and Nonthermal Effects. Nano Letters, 2018, 18, 1714-1723.	9.1	251
33	Direct Method for Optimized Effective Potentials in Density-Functional Theory. Physical Review Letters, 2002, 89, 143002.	7.8	250
34	Local softness and chemical reactivity in the molecules CO, SCNâ^' and H2CO. Computational and Theoretical Chemistry, 1988, 163, 305-313.	1.5	233
35	Quantum-Interference-Controlled Molecular Electronics. Nano Letters, 2008, 8, 3257-3261.	9.1	221
36	A chemical potential equalization method for molecular simulations. Journal of Chemical Physics, 1996, 104, 159-172.	3.0	219

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37	Fractional spins and static correlation error in density functional theory. Journal of Chemical Physics, 2008, 129, 121104.	3.0	215
38	Stochastic Voyages into Uncharted Chemical Space Produce a Representative Library of All Possible Drug-Like Compounds. Journal of the American Chemical Society, 2013, 135, 7296-7303.	13.7	214
39	Discontinuous Nature of the Exchange-Correlation Functional in Strongly Correlated Systems. Physical Review Letters, 2009, 102, 066403.	7.8	206
40	Electron transport through molecules:â€ƒSelf-consistent and non-self-consistent approaches. Physical Review B, 2004, 70, .	3.2	205
41	Self-interaction-free exchange-correlation functional for thermochemistry and kinetics. Journal of Chemical Physics, 2006, 124, 091102.	3.0	179
42	Linearâ€scaling semiempirical quantum calculations for macromolecules. Journal of Chemical Physics, 1996, 105, 2744-2750.	3.0	178
43	Toward the Accurate Modeling of DNA: The Importance of Long-Range Electrostatics. Journal of the American Chemical Society, 1995, 117, 5001-5002.	13.7	172
44	Activating MoS₂ for pH-Universal Hydrogen Evolution Catalysis. Journal of the American Chemical Society, 2017, 139, 16194-16200.	13.7	164
45	Improving Band Gap Prediction in Density Functional Theory from Molecules to Solids. Physical Review Letters, 2011, 107, 026403.	7.8	161
46	Delocalization errors in density functionals and implications for main-group thermochemistry. Journal of Chemical Physics, 2008, 129, 204112.	3.0	159
47	Accurate polymer polarizabilities with exact exchange density-functional theory. Journal of Chemical Physics, 2003, 119, 11001-11004.	3.0	154
48	Derivative discontinuity, bandgap and lowest unoccupied molecular orbital in density functional theory. Journal of Chemical Physics, 2012, 136, 204111.	3.0	154
49	Noncovalent Interaction Analysis in Fluctuating Environments. Journal of Chemical Theory and Computation, 2013, 9, 2226-2234.	5.3	150
50	Nature of ground and electronic excited states of higher acenes. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E5098-107.	7.1	147
51	Direct calculation of electron density in density-functional theory: Implementation for benzene and a tetrapeptide. Physical Review A, 1991, 44, 7823-7826.	2.5	140
52	Quantum mechanics simulation of protein dynamics on long timescale. Proteins: Structure, Function and Bioinformatics, 2001, 44, 484-489.	2.6	140
53	Designing Molecules by Optimizing Potentials. Journal of the American Chemical Society, 2006, 128, 3228-3232.	13.7	138
54	QM/MM Minimum Free-Energy Path:â€‰ Methodology and Application to Triosephosphate Isomerase. Journal of Chemical Theory and Computation, 2007, 3, 390-406.	5.3	135

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55	Gradient correction in Thomas-Fermi theory. Physical Review A, 1986, 34, 4575-4585.	2.5	132
56	Fitting Molecular Electrostatic Potentials from Quantum Mechanical Calculations. Journal of Chemical Theory and Computation, 2007, 3, 1004-1013.	5.3	125
57	The collocation method for bound solutions of the SchrÃ¶dinger equation. Chemical Physics Letters, 1988, 153, 98-104.	2.6	124
58	Perspective on "Density-functional theory for fractional particle number: derivative discontinuities of the energy". Theoretical Chemistry Accounts, 2000, 103, 346-348.	1.4	124
59	Near-perfect conduction through a ferrocene-based molecular wire. Physical Review B, 2005, 71, .	3.2	121
60	Density-functional theory (hyper)polarizabilities of push-pull Ï€-conjugated systems: Treatment of exact exchange and role of correlation. Journal of Chemical Physics, 2005, 123, 014319.	3.0	120
61	Nonorthogonal localized molecular orbitals in electronic structure theory. Journal of Chemical Physics, 2000, 112, 1634-1644.	3.0	119
62	Contact atomic structure and electron transport through molecules. Journal of Chemical Physics, 2005, 122, 074704.	3.0	119
63	Molecular softness as the average of atomic softnesses: companion principle to the geometric mean principle for electronegativity equalization. The Journal of Physical Chemistry, 1985, 89, 5412-5414.	2.9	118
64	Simultaneous-trajectory surface hopping: A parameter-free algorithm for implementing decoherence in nonadiabatic dynamics. Journal of Chemical Physics, 2011, 134, 144102.	3.0	117
65	Optimized Effective Potentials in Finite Basis Sets. Physical Review Letters, 2007, 98, 256401.	7.8	116
66	Absolute-energy-minimum principles for linear-scaling electronic-structure calculations. Physical Review B, 1997, 56, 9294-9297.	3.2	114
67	The fast Fourier Poisson method for calculating Ewald sums. Journal of Chemical Physics, 1994, 101, 3298-3300.	3.0	112
68	Organometallic Spintronics:Â Dicobaltocene Switch. Nano Letters, 2005, 5, 1959-1962.	9.1	112
69	Quantum mechanics/molecular mechanics minimum free-energy path for accurate reaction energetics in solution and enzymes: Sequential sampling and optimization on the potential of mean force surface. Journal of Chemical Physics, 2008, 128, 034105.	3.0	110
70	Molecular Dynamics Simulations with Quantum Mechanics/Molecular Mechanics and Adaptive Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 1442-1455.	5.3	110
71	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. National Science Review, 2018, 5, 203-215.	9.5	110
72	Various functionals for the kinetic energy density of an atom or molecule. Physical Review A, 1986, 34, 4586-4590.	2.5	107

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73	Shape of large single- and multiple-shell fullerenes. Physical Review B, 1994, 49, 11421-11424.	3.2	107
74	Singletâ^'Triplet Energy Gaps for Diradicals from Fractional-Spin Density-Functional Theory. Journal of Physical Chemistry A, 2011, 115, 76-83.	2.5	107
75	A Donorâ^'Nanotube Paradigm for Nonlinear Optical Materials. Nano Letters, 2008, 8, 2814-2818.	9.1	106
76	Coupling Quantum Interpretative Techniques: Another Look at Chemical Mechanisms in Organic Reactions. Journal of Chemical Theory and Computation, 2012, 8, 3993-3997.	5.3	104
77	How Is the Active Site of Enolase Organized To Catalyze Two Different Reaction Steps?. Journal of the American Chemical Society, 2000, 122, 6560-6570.	13.7	103
78	Role of the exchange-correlation potential in ab initio electron transport calculations. Journal of Chemical Physics, 2007, 126, 201102.	3.0	103
79	Molecular Design of Porphyrin-Based Nonlinear Optical Materials. Journal of Physical Chemistry A, 2008, 112, 12203-12207.	2.5	100
80	Orbital-dependent correlation energy in density-functional theory based on a second-order perturbation approach: Success and failure. Journal of Chemical Physics, 2005, 123, 062204.	3.0	99
81	Engineering Substrate Interaction To Improve Hydrogen Evolution Catalysis of Monolayer MoS₂ Films beyond Pt. ACS Nano, 2020, 14, 1707-1714.	14.6	97
82	Single-Molecule Conductance of Pyridine-Terminated Dithienylethene Switch Molecules. ACS Nano, 2011, 5, 5115-5123.	14.6	95
83	Phase-corrected surface hopping: Correcting the phase evolution of the electronic wavefunction. Journal of Chemical Physics, 2011, 135, 024101.	3.0	95
84	Potential Functionals: Dual to Density Functionals and Solution to thev-Representability Problem. Physical Review Letters, 2004, 92, 146404.	7.8	94
85	Multiscale Quantum Mechanics/Molecular Mechanics Simulations with Neural Networks. Journal of Chemical Theory and Computation, 2016, 12, 4934-4946.	5.3	94
86	Density-functional theory calculations with correct long-range potentials. Journal of Chemical Physics, 2003, 119, 2978-2990.	3.0	93
87	Quadratic string method for determining the minimum-energy path based on multiobjective optimization. Journal of Chemical Physics, 2006, 124, 054109.	3.0	93
88	The Arâ€“C2H2 intermolecular potential from high resolution spectroscopy and ab initio theory: A case for multicenter interactions. Journal of Chemical Physics, 1993, 99, 8585-8598.	3.0	92
89	Molecular Conductance:Â Chemical Trends of Anchoring Groups. Journal of the American Chemical Society, 2004, 126, 15897-15904.	13.7	92
90	Thermopower of Molecular Junctions: An ab Initio Study. Nano Letters, 2009, 9, 1011-1014.	9.1	91

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91	Ab Initio QM/MM Study Shows There Is No General Acid in the Reaction Catalyzed by 4-Oxalocrotonate Tautomerase. Journal of the American Chemical Society, 2003, 125, 10384-10393.	13.7	89
92	ALGEBRAIC EQUATION AND ITERATIVE OPTIMIZATION FOR THE OPTIMIZED EFFECTIVE POTENTIAL IN DENSITY FUNCTIONAL THEORY. Journal of Theoretical and Computational Chemistry, 2003, 02, 627-638.	1.8	82
93	Models of electrodes and contacts in molecular electronics. Journal of Chemical Physics, 2005, 123, 114701.	3.0	79
94	Simulating Water with the Self-Consistent-Charge Density Functional Tight Binding Method:Â From Molecular Clusters to the Liquid Stateâ€. Journal of Physical Chemistry A, 2007, 111, 5685-5691.	2.5	79
95	Development and application of ab initio QM/MM methods for mechanistic simulation of reactions in solution and in enzymes. Computational and Theoretical Chemistry, 2009, 898, 17-30.	1.5	78
96	Exchange-correlation energy from pairing matrix fluctuation and the particle-particle random-phase approximation. Physical Review A, 2013, 88, .	2.5	78
97	First-principles study of the structural and electronic properties of ethylene adsorption on Si(100)-(2Ã—1) surface. Journal of Chemical Physics, 1997, 107, 3981-3985.	3.0	77
98	Generalized adiabatic connection in density functional theory. Journal of Chemical Physics, 1998, 109, 10107-10110.	3.0	77
99	Using Density Functional Theory To Design DNA Base Analogues with Low Oxidation Potentials. Journal of Physical Chemistry B, 2001, 105, 6437-6444.	2.6	75
100	Negative Differential Resistance and Hysteresis through an Organometallic Molecule from Molecular-Level Crossing. Journal of the American Chemical Society, 2006, 128, 6274-6275.	13.7	71
101	Organometallic molecular rectification. Journal of Chemical Physics, 2006, 124, 024718.	3.0	71
102	Accelerating self-consistent field convergence with the augmented Roothaanâ€“Hall energy function. Journal of Chemical Physics, 2010, 132, 054109.	3.0	69
103	Local Scaling Correction for Reducing Delocalization Error in Density Functional Approximations. Physical Review Letters, 2015, 114, 053001.	7.8	69
104	Electron density as the basic variable: a divide-and-conquer approach to the ab initio computation of large molecules. Computational and Theoretical Chemistry, 1992, 255, 461-479.	1.5	68
105	Analytical energy gradients and geometry optimization in the divideâ€andâ€conquer method for large molecules. Journal of Chemical Physics, 1995, 102, 9598-9603.	3.0	68
106	Adapting the nudged elastic band method for determining minimum-energy paths of chemical reactions in enzymes. Journal of Chemical Physics, 2004, 120, 8039-8052.	3.0	67
107	Analytical evaluation of Fukui functions and real-space linear response function. Journal of Chemical Physics, 2012, 136, 144110.	3.0	67
108	Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains. Journal of Chemical Physics, 2012, 137, 214106.	3.0	66

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109	Quantum Mechanical Treatment of Biological Macromolecules in Solution Using Linear-Scaling Electronic Structure Methods. Physical Review Letters, 1998, 80, 5011-5014.	7.8	65
110	The collocation method for calculating vibrational bound states of molecular systemsâ€"with application to Arâ€"HCl. Journal of Chemical Physics, 1989, 90, 1746-1751.	3.0	64
111	The Protein Backbone Makes Important Contributions to 4-Oxalocrotonate Tautomerase Enzyme Catalysis:Â Understanding from Theory and Experimentâ€. Biochemistry, 2004, 43, 6885-6892.	2.5	64
112	Structural manifestation of the delocalization error of density functional approximations: C4N+2 rings and C20 bowl, cage, and ring isomers. Journal of Chemical Physics, 2010, 132, 234113.	3.0	63
113	Quantum Mechanical Study of Aqueous Polarization Effects on Biological Macromolecules. Journal of the American Chemical Society, 1996, 118, 10940-10941.	13.7	61
114	Ab initio quantum mechanical/molecular mechanical simulation of electron transfer process: Fractional electron approach. Journal of Chemical Physics, 2008, 128, 124510.	3.0	61
115	Second-Order Perturbation Theory with Fractional Charges and Fractional Spins. Journal of Chemical Theory and Computation, 2009, 5, 786-792.	5.3	61
116	Legendre-transform functionals for spin-density-functional theory. Journal of Chemical Physics, 2006, 124, 224108.	3.0	60
117	Density functional theory investigation of the polarizability and second hyperpolarizability of polydiacetylene and polybutatriene chains: Treatment of exact exchange and role of correlation. Journal of Chemical Physics, 2006, 125, 194114.	3.0	59
118	Assessment and formal properties of exchange-correlation functionals constructed from the adiabatic connection. Journal of Chemical Physics, 2007, 127, 034101.	3.0	59
119	Reaction path potential for complex systems derived from combined ab initio quantum mechanical and molecular mechanical calculations. Journal of Chemical Physics, 2004, 121, 89.	3.0	57
120	Strategy To Discover Diverse Optimal Molecules in the Small Molecule Universe. Journal of Chemical Information and Modeling, 2015, 55, 529-537.	5.4	57
121	The divideâ€andâ€conquer densityâ€functional approach: Molecular internal rotation and density of states. Journal of Chemical Physics, 1992, 96, 2408-2411.	3.0	56
122	Density-functional calculations of the structure and stability ofC240. Physical Review B, 1994, 49, 8526-8528.	3.2	56
123	Predicting the Frequency Dispersion of Electronic Hyperpolarizabilities on the Basis of Absorption Data and Thomasâ"Kuhn Sum Rules. Journal of Physical Chemistry C, 2010, 114, 2349-2359.	3.1	56
124	Describing strong correlation with fractional-spin correction in density functional theory. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9678-9683.	7.1	56
125	Parameterization and efficient implementation of a solvent model for linear-scaling semiempirical quantum mechanical calculations of biological macromolecules. Chemical Physics Letters, 1996, 263, 297-304.	2.6	55
126	Double, Rydberg and charge transfer excitations from pairing matrix fluctuation and particle-particle random phase approximation. Journal of Chemical Physics, 2013, 139, 224105.	3.0	52

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127	Intermolecular effect in molecular electronics. Journal of Chemical Physics, 2005, 122, 044703.	3.0	51
128	Direct Detection of the Formation of V-Amylose Helix by Single Molecule Force Spectroscopy. Journal of the American Chemical Society, 2006, 128, 9387-9393.	13.7	51
129	Failure of the random-phase-approximation correlation energy. Physical Review A, 2012, 85, .	2.5	51
130	Theoretical study of catalytic mechanism for single-site water oxidation process. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15669-15672.	7.1	51
131	Equivalence of particle-particle random phase approximation correlation energy and ladder-coupled-cluster doubles. Journal of Chemical Physics, 2013, 139, 104112.	3.0	51
132	An adapted form of the collocation method for calculating energy levels of rotating atomâ€“diatom complexes. Journal of Chemical Physics, 1989, 91, 6598-6603.	3.0	50
133	Contact Transparency of Nanotube-Molecule-Nanotube Junctions. Physical Review Letters, 2007, 99, 146802.	7.8	50
134	Designing Molecules with Optimal Properties Using the Linear Combination of Atomic Potentials Approach in an AM1 Semiempirical Framework. Journal of Physical Chemistry A, 2007, 111, 176-181.	2.5	50
135	New relation between hardness and compressibility of minerals. Physics and Chemistry of Minerals, 1987, 15, 191-195.	0.8	49
136	Nuclear quantum effects on an enzyme-catalyzed reaction with reaction path potential: Proton transfer in triosephosphate isomerase. Journal of Chemical Physics, 2006, 124, 124516.	3.0	49
137	Fast evaluation of the Coulomb energy for electron densities. Journal of Chemical Physics, 1997, 107, 1218-1226.	3.0	48
138	Optimized effective potentials from electron densities in finite basis sets. Journal of Chemical Physics, 2007, 127, 174101.	3.0	48
139	Cobaltocene as a spin filter. Journal of Chemical Physics, 2007, 127, 141104.	3.0	47
140	A new functional with homogeneous coordinate scaling in density functional theory: Fâ€‰[â€‰ï¸¡Î»]. Journal of Chemical Physics, 1985, 83, 2334-2336.	3.0	46
141	Force Field for Water Based on Neural Network. Journal of Physical Chemistry Letters, 2018, 9, 3232-3240.	4.6	46
142	Linear-scaling quantum mechanical calculations of biological molecules: The divide-and-conquer approach. Computational Materials Science, 1998, 12, 259-277.	3.0	45
143	Elastic Properties of Single Amylose Chains in Water:Â A Quantum Mechanical and AFM Study. Journal of the American Chemical Society, 2004, 126, 9033-9041.	13.7	45
144	Computational design, synthesis and biological evaluation of para-quinone-based inhibitors for redox regulation of the dual-specificity phosphatase Cdc25B. Organic and Biomolecular Chemistry, 2008, 6, 3256.	2.8	45

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145	Time-dependent transport through molecular junctions. Journal of Chemical Physics, 2010, 132, 234105.	3.0	45
146	Fractional Charge Behavior and Band Gap Predictions with the XYG3 Type of Doubly Hybrid Density Functionals. Journal of Physical Chemistry A, 2014, 118, 9201-9211.	2.5	45
147	An algorithm for 3D numerical integration that scales linearly with the size of the molecule. Chemical Physics Letters, 1995, 241, 469-476.	2.6	44
148	A concise redefinition of the solid spherical harmonics and its use in fast multipole methods. Journal of Chemical Physics, 1996, 104, 8003-8006.	3.0	44
149	Electron transport through molecules: Gate-induced polarization and potential shift. Physical Review B, 2005, 71, .	3.2	44
150	Achieving partial decoherence in surface hopping through phase correction. Journal of Chemical Physics, 2012, 137, 22A528.	3.0	44
151	Parallel iterative reaction path optimization in ab initio quantum mechanical/molecular mechanical modeling of enzyme reactions. Journal of Chemical Physics, 2004, 121, 697-706.	3.0	43
152	Experimental Validation of the Docking Orientation of Cdc25 with Its Cdk2â^'CycA Protein Substrateâ€. Biochemistry, 2005, 44, 16563-16573.	2.5	43
153	Electron transport through single conjugated organic molecules: Basis set effects in ab initio calculations. Journal of Chemical Physics, 2007, 127, 144107.	3.0	43
154	Density-fragment interaction approach for quantum-mechanical/molecular-mechanical calculations with application to the excited states of a Mg2+-sensitive dye. Journal of Chemical Physics, 2008, 129, 054102.	3.0	43
155	Coarse-grained modeling of allosteric regulation in protein receptors. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 14253-14258.	7.1	43
156	A method for calculating vibrational bound states: Iterative solution of the collocation equations constructed from localized basis sets. Journal of Chemical Physics, 1990, 92, 522-526.	3.0	41
157	A local projection method for the linear combination of atomic orbital implementation of densityâ€functional theory. Journal of Chemical Physics, 1991, 94, 1208-1214.	3.0	41
158	Mechanism of OMP Decarboxylation in Orotidine 5â€²-Monophosphate Decarboxylase. Journal of the American Chemical Society, 2008, 130, 14493-14503.	13.7	41
159	Sulfur-doped zinc oxide (ZnO) Nanostars: Synthesis and simulation of growth mechanism. Nano Research, 2012, 5, 20-26.	10.4	41
160	Benchmark tests and spin adaptation for the particle-particle random phase approximation. Journal of Chemical Physics, 2013, 139, 174110.	3.0	40
161	Excitation energies from particle-particle random phase approximation: Davidson algorithm and benchmark studies. Journal of Chemical Physics, 2014, 141, 124104.	3.0	40
162	A gradient-directed Monte Carlo approach to molecular design. Journal of Chemical Physics, 2008, 129, 064102.	3.0	39

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163	Optimized effective potentials from arbitrary basis sets. Journal of Chemical Physics, 2008, 129, 194102.	3.0	39
164	Active Species for the Ground-State Complex of Cytidine Deaminase:â€‰ A Linear-Scaling Quantum Mechanical Investigation. Journal of the American Chemical Society, 1998, 120, 5407-5410.	13.7	38
165	Conjugate-gradient optimization method for orbital-free density functional calculations. Journal of Chemical Physics, 2004, 121, 2030-2036.	3.0	38
166	Higher-order split operator schemes for solving the SchrÃ¶dinger equation in the time-dependent wave packet method: applications to triatomic reactive scattering calculations. Physical Chemistry Chemical Physics, 2012, 14, 1827.	2.8	38
167	Fukui Function. , 2009, , .		37
168	Reaction path determination for quantum mechanical/molecular mechanical modeling of enzyme reactions by combining first order and second order â€œchain-of-replicasâ€•methods. Journal of Chemical Physics, 2005, 122, 114502.	3.0	36
169	Exploring chemical space with discrete, gradient, and hybrid optimization methods. Journal of Chemical Physics, 2008, 129, 174105.	3.0	36
170	Full Reconstruction of a Vectorial Protein Folding Pathway by Atomic Force Microscopy and Molecular Dynamics Simulations*. Journal of Biological Chemistry, 2010, 285, 38167-38172.	3.4	36
171	Autocatalytic Intramolecular Isopeptide Bond Formation in Gram-Positive Bacterial Pili: A QM/MM Simulation. Journal of the American Chemical Society, 2011, 133, 478-485.	13.7	36
172	Inverse molecular design in a tight-binding framework. Journal of Chemical Physics, 2008, 129, 044106.	3.0	35
173	Calculating solution redox free energies with ab initio quantum mechanical/molecular mechanical minimum free energy path method. Journal of Chemical Physics, 2009, 130, 164111.	3.0	35
174	Exchange-correlation energy from pairing matrix fluctuation and the particle-particle random phase approximation. Journal of Chemical Physics, 2014, 140, 18A511.	3.0	34
175	Singletâ€“Triplet Energy Gaps for Diradicals from Particleâ€“Particle Random Phase Approximation. Journal of Physical Chemistry A, 2015, 119, 4923-4932.	2.5	34
176	Design of Coupled Porphyrin Chromophores with Unusually Large Hyperpolarizabilities. Journal of Physical Chemistry C, 2012, 116, 9724-9733.	3.1	33
177	Describing Chemical Reactivity with Frontier Molecular Orbitalets. Jacs Au, 2022, 2, 1383-1394.	7.9	32
178	A pseudobond parametrization for improved electrostatics in quantum mechanical/molecular mechanical simulations of enzymes. Journal of Chemical Physics, 2008, 129, 154106.	3.0	31
179	Chaperones Rescue Luciferase Folding by Separating Its Domains. Journal of Biological Chemistry, 2014, 289, 28607-28618.	3.4	31
180	Preserving Symmetry and Degeneracy in the Localized Orbital Scaling Correction Approach. Journal of Physical Chemistry Letters, 2020, 11, 1528-1535.	4.6	31

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181	Ab initioapproach for many-electron systems without invoking orbitals: An integral formulation of density-functional theory. Physical Review Letters, 1987, 59, 1569-1572.	7.8	30
182	Density-functional theory simulation of large quantum dots. Physical Review B, 2003, 68, .	3.2	30
183	Linear-response time-dependent density-functional theory with pairing fields. Journal of Chemical Physics, 2014, 140, 18A522.	3.0	30
184	Dual-topology/dual-coordinate free-energy simulation using QM/MM force field. Journal of Chemical Physics, 2005, 123, 041102.	3.0	29
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