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	Multireference Density Functional Theory for Describing Ground and Excited States with Renormalized Singles. Journal of Physical Chemistry Letters, 2022, 13, 894-903.	4.6	8
2	LibSC: Library for Scaling Correction Methods in Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 840-850.	5.3	8
3	Combining Localized Orbital Scaling Correction and Bethe-Salpeter Equation for Accurate Excitation Energies. Journal of Chemical Physics, 2022, 156, 154101.	3.0	6
4	Reformulation of thermally assisted-occupation density functional theory in the Kohn–Sham framework. Journal of Chemical Physics, 2022, 156, 174108.	3.0	6
5	Regularized Localized Molecular Orbitals in a Divide-and-Conquer Approach for Linear Scaling Calculations. Journal of Chemical Theory and Computation, 2022, 18, 2975-2982.	5.3	3
6	Describing Chemical Reactivity with Frontier Molecular Orbitalets. Jacs Au, 2022, 2, 1383-1394.	7.9	32
7	Describing polymer polarizability with localized orbital scaling correction in density functional theory. Journal of Chemical Physics, 2021, 154, 054302.	3.0	11
8	Exact Second-Order Corrections and Accurate Quasiparticle Energy Calculations in Density Functional Theory. Journal of Physical Chemistry Letters, 2021, 12, 7236-7244.	4.6	8
9	Renormalized Singles Green's Function in the T-Matrix Approximation for Accurate Quasiparticle Energy Calculation. Journal of Physical Chemistry Letters, 2021, 12, 6203-6210.	4.6	19
10	Mechanism of Reduction of an Aminyl Radical Intermediate in the Radical SAM GTP 3′,8-Cyclase MoaA. Journal of the American Chemical Society, 2021, 143, 13835-13844.	13.7	7
11	Theoretical Studies on Triplet-state Driven Dissociation of Formaldehyde by Quasi-classical Molecular Dynamics Simulation on Machine-Learning Potential Energy Surface. Journal of Chemical Physics, 2021, 155, 214105.	3.0	3
12	Self-Consistent Calculation of the Localized Orbital Scaling Correction for Correct Electron Densities and Energy-Level Alignments in Density Functional Theory. Journal of Physical Chemistry Letters, 2020, 11, 10269-10277.	4.6	18
13	Piecewise All-Atom SMD Simulations Reveal Key Secondary Structures in Luciferase Unfolding Pathway. Biophysical Journal, 2020, 119, 2251-2261.	0.5	3
14	Arene Substitution Design for Controlled Conformational Changes of Dibenzocycloocta-1,5-dienes. Journal of the American Chemical Society, 2020, 142, 16651-16660.	13.7	11
15	Introductory lecture: when the density of the noninteracting reference system is not the density of the physical system in density functional theory. Faraday Discussions, 2020, 224, 9-26.	3.2	6
16	Cobalt(II)‐Catalyzed [4+2] Annulation of Picolinamides with Alkynes via C–H Bond Activation. Chemistry - A European Journal, 2020, 26, 5607-5610.	3.3	11
17	Engineering Substrate Interaction To Improve Hydrogen Evolution Catalysis of Monolayer MoS_2 Films beyond Pt. ACS Nano, 2020, 14, 1707-1714.	14.6	97
18	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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19	Mechanism of Rate Acceleration of Radical C–C Bond Formation Reaction by a Radical SAM GTP 3′,8-Cyclase. Journal of the American Chemical Society, 2020, 142, 9314-9326.	13.7	15
20	Revisiting the Hole Size in Double Helical DNA with Localized Orbital Scaling Corrections. Journal of Physical Chemistry B, 2020, 124, 3428-3435.	2.6	5
21	Density Functional Prediction of Quasiparticle, Excitation, and Resonance Energies of Molecules With a Global Scaling Correction Approach. Frontiers in Chemistry, 2020, 8, 588808.	3.6	4
22	1,3-Dipolar cycloaddition of nitrones to oxa(aza)bicyclic alkenes. Organic Chemistry Frontiers, 2019, 6, 3360-3364.	4.5	19
23	Excited-State Potential Energy Surfaces, Conical Intersections, and Analytical Gradients from Ground-State Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 2538-2545.	4.6	23
24	Charge transfer excitation energies from ground state density functional theory calculations. Journal of Chemical Physics, 2019, 150, 144109.	3.0	10
25	Excitation Energies from the Single-Particle Green's Function with the GW Approximation. Journal of Physical Chemistry A, 2019, 123, 3199-3204.	2.5	7
26	Solvation Free Energy Calculations with Quantum Mechanics/Molecular Mechanics and Machine Learning Models. Journal of Physical Chemistry B, 2019, 123, 901-908.	2.6	25
27	Toward Building Protein Force Fields by Residue-Based Systematic Molecular Fragmentation and Neural Network. Journal of Chemical Theory and Computation, 2019, 15, 1409-1417.	5.3	18
28	Approximating Quasiparticle and Excitation Energies from Ground State Generalized Kohn–Sham Calculations. Journal of Physical Chemistry A, 2019, 123, 666-673.	2.5	26
29	Renormalized Singles Green's Function for Quasi-Particle Calculations beyond the G_0W_0 Approximation. Journal of Physical Chemistry Letters, 2019, 10, 447-452.	4.6	17
30	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
31	Plasmon-Enhanced Catalysis: Distinguishing Thermal and Nonthermal Effects. Nano Letters, 2018, 18, 1714-1723.	9.1	251
32	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. National Science Review, 2018, 5, 203-215.	9.5	110
33	Accurate density functional prediction of molecular electron affinity with the scaling corrected Kohn–Sham frontier orbital energies. Molecular Physics, 2018, 116, 927-934.	1.7	10
34	Spin-state energetics of iron(II) porphyrin from the particle-particle random phase approximation. European Physical Journal B, 2018, 91, 1.	1.5	5
35	Role of Conformational Fluctuations of Protein toward Methylation in DNA by Cytosine-5-methyltransferase. Journal of Chemical Theory and Computation, 2018, 14, 6679-6689.	5.3	3
36	Field Electron Emission Images Far Away from a Semi-Infinitely Long Emitter: A Multiscale Simulation. Journal of Physical Chemistry C, 2018, 122, 27754-27760.	3.1	2

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37	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
38	Accurate Treatment of Charge-Transfer Excitations and Thermally Activated Delayed Fluorescence Using the Particle–Particle Random Phase Approximation. Journal of Chemical Theory and Computation, 2018, 14, 3196-3204.	5.3	12
39	Force Field for Water Based on Neural Network. Journal of Physical Chemistry Letters, 2018, 9, 3232-3240.	4.6	46
40	Single, Double Electronic Excitations and Exciton Effective Conjugation Lengths in Ï€-Conjugated Systems. Journal of Physical Chemistry Letters, 2018, 9, 4029-4036.	4.6	6
41	Accurate Quantum Mechanical/Molecular Mechanical Calculations of Reduction Potentials in Azurin Variants. Journal of Chemical Theory and Computation, 2018, 14, 4948-4957.	5.3	15
42	Photocatalytic activity and the radiative lifetimes of excitons *via* an *ab initio* approach. Journal of Materials Chemistry A, 2018, 6, 15027-15032.	10.3	12
43	Perspective: Chemical Information Encoded in Electron Density. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2018, 34, 567-580.	4.9	4
44	Product selectivity in plasmonic photocatalysis for carbon dioxide hydrogenation. Nature Communications, 2017, 8, 14542.	12.8	348
45	Three Pyrimidine Decarboxylations in the Absence of a Catalyst. Biochemistry, 2017, 56, 1498-1503.	2.5	1
46	On the piecewise convex or concave nature of ground state energy as a function of fractional number of electrons for approximate density functionals. Journal of Chemical Physics, 2017, 146, 074107.	3.0	14
47	Understanding band gaps of solids in generalized Kohn–Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
48	Electron Density, Kohn–Sham Frontier Orbitals, and Fukui Functions. , 2017, , 303-306.		1
49	Competing Pathways and Multiple Folding Nuclei in a Large Multidomain Protein, Luciferase. Biophysical Journal, 2017, 112, 1829-1840.	0.5	12
50	On extending Kohn-Sham density functionals to systems with fractional number of electrons. Journal of Chemical Physics, 2017, 146, 214109.	3.0	5
51	Charge transfer excitations from particle-particle random phase approximation—Opportunities and challenges arising from two-electron deficient systems. Journal of Chemical Physics, 2017, 146, 124104.	3.0	10
52	Activating MoS_2 for pH-Universal Hydrogen Evolution Catalysis. Journal of the American Chemical Society, 2017, 139, 16194-16200.	13.7	164
53	Excitation energies from particle-particle random phase approximation with accurate optimized effective potentials. Journal of Chemical Physics, 2017, 147, 134105.	3.0	4
54	Multireference Density Functional Theory with Generalized Auxiliary Systems for Ground and Excited States. Journal of Physical Chemistry Letters, 2017, 8, 4479-4485.	4.6	21

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55	Generalized Optimized Effective Potential for Orbital Functionals and Self-Consistent Calculation of Random Phase Approximations. Journal of Physical Chemistry Letters, 2017, 8, 4746-4751.	4.6	18
56	Time-Dependent Coupled Perturbed Hartree–Fock and Density-Functional-Theory Approach for Calculating Frequency-Dependent (Hyper)Polarizabilities with Nonorthogonal Localized Molecular Orbitals. Journal of Chemical Theory and Computation, 2017, 13, 4101-4112.	5.3	1
57	Internal force corrections with machine learning for quantum mechanics/molecular mechanics simulations. Journal of Chemical Physics, 2017, 147, 161732.	3.0	28
58	Accurate Quasiparticle Spectra from the T-Matrix Self-Energy and the Particle–Particle Random Phase Approximation. Journal of Physical Chemistry Letters, 2017, 8, 3223-3227.	4.6	18
59	Single-molecule Force Spectroscopy Reveals the Calcium Dependence of the Alternative Conformations in the Native State of a $\gamma\beta$-Crystallin Protein. Journal of Biological Chemistry, 2016, 291, 18263-18275.	3.4	13
60	All The Catalytic Active Sites of MoS_2 for Hydrogen Evolution. Journal of the American Chemical Society, 2016, 138, 16632-16638.	13.7	664
61	Determining polarizable force fields with electrostatic potentials from quantum mechanical linear response theory. Journal of Chemical Physics, 2016, 144, 224107.	3.0	9
62	Accurate and efficient calculation of excitation energies with the active-space particle-particle random phase approximation. Journal of Chemical Physics, 2016, 145, 144105.	3.0	12
63	Quantum Mechanics/Molecular Mechanics Method Combined with Hybrid All-Atom and Coarse-Grained Model: Theory and Application on Redox Potential Calculations. Journal of Chemical Theory and Computation, 2016, 12, 2017-2027.	5.3	18
64	Direct Observation of Multimer Stabilization in the Mechanical Unfolding Pathway of a Protein Undergoing Oligomerization. Biophysical Journal, 2016, 110, 392a-393a.	0.5	0
65	Single-Molecule Force-Spectroscopy Reveals the Calcium Dependency of Folding Intermediates in the Multidomain Protein S. Biophysical Journal, 2016, 110, 393a.	0.5	0
66	Multiscale Quantum Mechanics/Molecular Mechanics Simulations with Neural Networks. Journal of Chemical Theory and Computation, 2016, 12, 4934-4946.	5.3	94
67	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
68	Conical Intersections from Particle–Particle Random Phase and Tamm–Dancoff Approximations. Journal of Physical Chemistry Letters, 2016, 7, 2407-2411.	4.6	23
69	Diverse Optimal Molecular Libraries for Organic Light-Emitting Diodes. Journal of Chemical Theory and Computation, 2016, 12, 1942-1952.	5.3	15
70	Accurate atomic quantum defects from particle–particle random phase approximation. Molecular Physics, 2016, 114, 1189-1198.	1.7	4
71	Gentlest ascent dynamics for calculating first excited state and exploring energy landscape of Kohn-Sham density functionals. Journal of Chemical Physics, 2015, 143, 224110.	3.0	7
72	Orbital relaxation effects on Kohn–Sham frontier orbital energies in density functional theory. Journal of Chemical Physics, 2015, 142, 154113.	3.0	18

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73	Angular momentum dependent field emission energy distribution. , 2015, , .		0
74	Local Scaling Correction for Reducing Delocalization Error in Density Functional Approximations. Physical Review Letters, 2015, 114, 053001.	7.8	69
75	Coupled-Perturbed SCF Approach for Calculating Static Polarizabilities and Hyperpolarizabilities with Nonorthogonal Localized Molecular Orbitals. Journal of Chemical Theory and Computation, 2015, 11, 923-931.	5.3	2
76	Direct Observation of Multimer Stabilization in the Mechanical Unfolding Pathway of a Protein Undergoing Oligomerization. ACS Nano, 2015, 9, 1189-1197.	14.6	18
77	Strategy To Discover Diverse Optimal Molecules in the Small Molecule Universe. Journal of Chemical Information and Modeling, 2015, 55, 529-537.	5.4	57
78	Singletâ€"Triplet Energy Gaps for Diradicals from Particleâ€"Particle Random Phase Approximation. Journal of Physical Chemistry A, 2015, 119, 4923-4932.	2.5	34
79	Scaling correction approaches for reducing delocalization error in density functional approximations. Science China Chemistry, 2015, 58, 1825-1844.	8.2	12
80	Analytic gradients, geometry optimization and excited state potential energy surfaces from the particle-particle random phase approximation. Physical Chemistry Chemical Physics, 2015, 17, 1025-1038.	2.8	21
81	A tribute to Guosen Yan. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	0
82	Restricted second random phase approximations and Tamm-Dancoff approximations for electronic excitation energy calculations. Journal of Chemical Physics, 2014, 141, 214102.	3.0	4
83	Exchange-correlation energy from pairing matrix fluctuation and the particle-particle random phase approximation. Journal of Chemical Physics, 2014, 140, 18A511.	3.0	34
84	Excitation energies from particle-particle random phase approximation: Davidson algorithm and benchmark studies. Journal of Chemical Physics, 2014, 141, 124104.	3.0	40
85	Tensor hypercontracted ppRPA: Reducing the cost of the particle-particle random phase approximation from $O(r^6)$ to $O(r^4)$. Journal of Chemical Physics, 2014, 141, 024119.	3.0	20
86	Chaperones Rescue Luciferase Folding by Separating Its Domains. Journal of Biological Chemistry, 2014, 289, 28607-28618.	3.4	31
87	Linear-response time-dependent density-functional theory with pairing fields. Journal of Chemical Physics, 2014, 140, 18A522.	3.0	30
88	Characterization of a Photoswitching Chelator with Light-Modulated Geometric, Electronic, and Metal-Binding Properties. Inorganic Chemistry, 2014, 53, 1397-1405.	4.0	23
89	Layer-Dependent Electrocatalysis of MoS_2 for Hydrogen Evolution. Nano Letters, 2014, 14, 553-558.	9.1	667
90	Shifting Electronic Structure by Inherent Tension in Molecular Bottlebrushes with Polythiophene Backbones. ACS Macro Letters, 2014, 3, 738-742.	4.8	16

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91	Revisiting H_2O Nucleation around Au^+ and Hg^{2+}: The Peculiar "Pseudo-Soft" Character of the Gold Cation. Journal of Chemical Theory and Computation, 2014, 10, 1900-1909.	5.3	7
92	Preface: Special Topic on Advances in Density Functional Theory. Journal of Chemical Physics, 2014, 140, 18A101.	3.0	6
93	Testing exchange–correlation functionals at fractional electron numbers. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	2
94	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
95	N-Terminal Domain of Luciferase Controls Misfolding Avoidance. Biophysical Journal, 2014, 106, 471a.	0.5	0
96	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
97	Effective preconditioning for ab initio ground state energy minimization with non-orthogonal localized molecular orbitals. Physical Chemistry Chemical Physics, 2013, 15, 15518.	2.8	13
98	Concerted Proton Transfer Mechanism of *Clostridium thermocellum* Ribose-5-phosphate Isomerase. Journal of Physical Chemistry B, 2013, 117, 9354-9361.	2.6	8
99	Exchange-correlation energy from pairing matrix fluctuation and the particle-particle random-phase approximation. Physical Review A, 2013, 88, .	2.5	78
100	A nonempirical scaling correction approach for density functional methods involving substantial amount of Hartree–Fock exchange. Journal of Chemical Physics, 2013, 138, 174105.	3.0	23
101	The tensor hypercontracted parametric reduced density matrix algorithm: Coupled-cluster accuracy with O(r4) scaling. Journal of Chemical Physics, 2013, 139, 054110.	3.0	20
102	Wave function methods for fractional electrons. Journal of Chemical Physics, 2013, 139, 074107.	3.0	19
103	Equivalence of particle-particle random phase approximation correlation energy and ladder-coupled-cluster doubles. Journal of Chemical Physics, 2013, 139, 104112.	3.0	51
104	Extension of many-body theory and approximate density functionals to fractional charges and fractional spins. Journal of Chemical Physics, 2013, 139, 104114.	3.0	29
105	Improving Single Molecule Force Spectroscopy through Automated Real-Time Data Collection and Quantification of Experimental Conditions. Biophysical Journal, 2013, 104, 512a.	0.5	0
106	Noncovalent Interaction Analysis in Fluctuating Environments. Journal of Chemical Theory and Computation, 2013, 9, 2226-2234.	5.3	150
107	Pushing the Boundaries of Intrinsically Stable Radicals: Inverse Design Using the Thiadiazinyl Radical as a Template. Journal of Organic Chemistry, 2013, 78, 3151-3158.	3.2	22
108	Fukui function and response function for nonlocal and fractional systems. Journal of Chemical Physics, 2013, 138, 184108.	3.0	18

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109	Dynamical second-order Bethe-Salpeter equation kernel: A method for electronic excitation beyond the adiabatic approximation. Journal of Chemical Physics, 2013, 139, 154109.	3.0	23
110	Accurate Computation of the Non-Interacting Kinetic Energy from Electron Densities. Recent Advances in Computational, 2013, , 13-29.	0.8	0
111	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
112	Pseudobond parameters for QM/MM studies involving nucleosides, nucleotides, and their analogs. Journal of Chemical Physics, 2013, 138, 045102.	3.0	5
113	Contributions of pauli repulsions to the energetics and physical properties computed in QM/MM methods. Journal of Computational Chemistry, 2013, 34, 2380-2388.	3.3	9
114	Benchmark tests and spin adaptation for the particle-particle random phase approximation. Journal of Chemical Physics, 2013, 139, 174110.	3.0	40
115	Failure of the random-phase-approximation correlation energy. Physical Review A, 2012, 85, .	2.5	51
116	Achieving partial decoherence in surface hopping through phase correction. Journal of Chemical Physics, 2012, 137, 22A528.	3.0	44
117	Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains. Journal of Chemical Physics, 2012, 137, 214106.	3.0	66
118	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
119	Optimized effective potential for calculations with orbital-free potential functionals. Molecular Physics, 2012, 110, 925-934.	1.7	3
120	Insight and progress in density functional theory. AIP Conference Proceedings, 2012, , .	0.4	3
121	Fragment-Based Quantum Mechanical/Molecular Mechanical Simulations of Thermodynamic and Kinetic Process of the Ru^{2+}–Ru^{3+} Self-Exchange Electron Transfer. Journal of Chemical Theory and Computation, 2012, 8, 4960-4967.	5.3	18
122	Variational fractional-spin density-functional theory for diradicals. Journal of Chemical Physics, 2012, 137, 114112.	3.0	27
123	Higher-order split operator schemes for solving the Schrödinger equation in the time-dependent wave packet method: applications to triatomic reactive scattering calculations. Physical Chemistry Chemical Physics, 2012, 14, 1827.	2.8	38
124	Liquid water simulations with the density fragment interaction approach. Physical Chemistry Chemical Physics, 2012, 14, 7700.	2.8	14
125	Design of Coupled Porphyrin Chromophores with Unusually Large Hyperpolarizabilities. Journal of Physical Chemistry C, 2012, 116, 9724-9733.	3.1	33
126	Catalytic Mechanism of 4-Oxalocrotonate Tautomerase: Significances of Protein–Protein Interactions on Proton Transfer Pathways. Journal of Physical Chemistry B, 2012, 116, 6889-6897.	2.6	7

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127	Density-Functional Errors in Alkanes: A Real-Space Perspective. Journal of Chemical Theory and Computation, 2012, 8, 2676-2681.	5.3	16
128	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
129	Analytical evaluation of Fukui functions and real-space linear response function. Journal of Chemical Physics, 2012, 136, 144110.	3.0	67
130	Derivative discontinuity, bandgap and lowest unoccupied molecular orbital in density functional theory. Journal of Chemical Physics, 2012, 136, 204111.	3.0	154
131	Mechanical Anisotropy of Ankyrin Repeats. Biophysical Journal, 2012, 102, 1118-1126.	0.5	20
132	Highly tunable spin-dependent electron transport through carbon atomic chains connecting two zigzag graphene nanoribbons. Journal of Chemical Physics, 2012, 137, 104107.	3.0	19
133	Inverse design of molecules with optimal reactivity properties: acidity of 2-naphthol derivatives. Physical Chemistry Chemical Physics, 2012, 14, 16002.	2.8	24
134	Challenges for Density Functional Theory. Chemical Reviews, 2012, 112, 289-320.	47.7	1,869
135	Sulfur-doped zinc oxide (ZnO) Nanostars: Synthesis and simulation of growth mechanism. Nano Research, 2012, 5, 20-26.	10.4	41
136	Single-Molecule Conductance of Pyridine-Terminated Dithienylethene Switch Molecules. ACS Nano, 2011, 5, 5115-5123.	14.6	95
137	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
138	Improving Band Gap Prediction in Density Functional Theory from Molecules to Solids. Physical Review Letters, 2011, 107, 026403.	7.8	161
139	Î»-Metadynamics Approach To Compute Absolute Solvation Free Energy. Journal of Physical Chemistry Letters, 2011, 2, 2099-2103.	4.6	24
140	Phase-corrected surface hopping: Correcting the phase evolution of the electronic wavefunction. Journal of Chemical Physics, 2011, 135, 024101.	3.0	95
141	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
142	Conical intersections in solution: Formulation, algorithm, and implementation with combined quantum mechanics/molecular mechanics method. Journal of Chemical Physics, 2011, 134, 204115.	3.0	14
143	Singletâˆ'Triplet Energy Gaps for Diradicals from Fractional-Spin Density-Functional Theory. Journal of Physical Chemistry A, 2011, 115, 76-83.	2.5	107
144	NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	5.3	2,897

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145	Simultaneous-trajectory surface hopping: A parameter-free algorithm for implementing decoherence in nonadiabatic dynamics. Journal of Chemical Physics, 2011, 134, 144102.	3.0	117
146	Communication: An exact short-time solver for the time-dependent Schrödinger equation. Journal of Chemical Physics, 2011, 134, 041101.	3.0	15
147	An algebraic operator approach to electronic structure. Journal of Chemical Physics, 2011, 135, 244111.	3.0	0
148	Accelerating self-consistent field convergence with the augmented Roothaan–Hall energy function. Journal of Chemical Physics, 2010, 132, 054109.	3.0	69
149	Revealing Noncovalent Interactions. Journal of the American Chemical Society, 2010, 132, 6498-6506.	13.7	6,465
150	Synthesis and chemical diversity analysis of bicyclo[3.3.1]non-3-en-2-ones. Tetrahedron, 2010, 66, 5852-5862.	1.9	17
151	A gradient–directed Monte Carlo approach for protein design. Journal of Computational Chemistry, 2010, 31, 2164-2168.	3.3	12
152	Concerted O atom–proton transfer in the O–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
153	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
154	Spin-state splittings, highest-occupied-molecular-orbital and lowest-unoccupied-molecular-orbital energies, and chemical hardness. Journal of Chemical Physics, 2010, 133, 164107.	3.0	14
155	Efficient Construction of Nonorthogonal Localized Molecular Orbitals in Large Systems[–]. Journal of Physical Chemistry A, 2010, 114, 8878-8883.	2.5	10
156	Conductive junctions with parallel graphene sheets. Journal of Chemical Physics, 2010, 132, 114703.	3.0	11
157	Equilibrium Sampling for Biomolecules under Mechanical Tension. Biophysical Journal, 2010, 98, 733-740.	0.5	6
158	Predicting the Frequency Dispersion of Electronic Hyperpolarizabilities on the Basis of Absorption Data and Thomas–Kuhn Sum Rules. Journal of Physical Chemistry C, 2010, 114, 2349-2359.	3.1	56
159	Challenges with range-separated exchange-correlation functionals in time-dependent density functional theory calculations. Molecular Physics, 2010, 108, 2745-2750.	1.7	20
160	Elucidating Solvent Contributions to Solution Reactions with Ab Initio QM/MM Methods. Journal of Physical Chemistry B, 2010, 114, 2755-2759.	2.6	16
161	Time-dependent transport through molecular junctions. Journal of Chemical Physics, 2010, 132, 234105.	3.0	45
162	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

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163	Reformulating time-dependent density functional theory with non-orthogonal localized molecular orbitals. Physical Chemistry Chemical Physics, 2010, 12, 416-421.	2.8	26
164	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
165	A gradient-directed Monte Carlo method for global optimization in a discrete space: Application to protein sequence design and folding. Journal of Chemical Physics, 2009, 131, 154117.	3.0	15
166	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
167	Emergent strategies for inverse molecular design. Science in China Series B: Chemistry, 2009, 52, 1769-1776.	0.8	9
168	Analysis of HIF-1 inhibition by manassantin A and analogues with modified tetrahydrofuran configurations. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3783-3786.	2.2	24
169	Discrete Optimization of Electronic Hyperpolarizabilities in a Chemical Subspace. Journal of Chemical Theory and Computation, 2009, 5, 3321-3329.	5.3	21
170	Discontinuous Nature of the Exchange-Correlation Functional in Strongly Correlated Systems. Physical Review Letters, 2009, 102, 066403.	7.8	206
171	Mechanism of Cdc25B Phosphatase with the Small Molecule Substrate p-Nitrophenyl Phosphate from QM/MM-MFEP Calculations. Journal of Physical Chemistry B, 2009, 113, 5217-5224.	2.6	25
172	Thermopower of Molecular Junctions: An ab Initio Study. Nano Letters, 2009, 9, 1011-1014.	9.1	91
173	Contact Geometry and Conductance of Crossed Nanotube Junctions under Pressure. Nano Letters, 2009, 9, 1759-1763.	9.1	9
174	Second-Order Perturbation Theory with Fractional Charges and Fractional Spins. Journal of Chemical Theory and Computation, 2009, 5, 786-792.	5.3	61
175	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
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