Donald G Truhlar

List of Publications by Year
in descending order

1,408	184,323	73	63
papers	citations	h-index	g-index

1522	1522	1522	62053
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. Theoretical Chemistry Accounts, 2008, 120, 215-241.	0.5	23,928
2	Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. Journal of Physical Chemistry B, 2009, 113, 6378-6396.	1.2	12,475
3	Density Functionals with Broad Applicability in Chemistry. Accounts of Chemical Research, 2008, 41, 157-167.	7.6	6,193
4	A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. Journal of Chemical Physics, 2006, 125, 194101.	1.2	4,175
5	Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2006, 2, 364-382.	2.3	3,329
6	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
7	Implicit Solvation Models:â€‰ Equilibria, Structure, Spectra, and Dynamics. Chemical Reviews, 1999, 99, 2161-2200.	23.0	2,123
8	Current Status of Transition-State Theory. The Journal of Physical Chemistry, 1996, 100, 12771-12800.	2.9	1,795
9	Hybrid Meta Density Functional Theory Methods for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions:â€‰ The MPW1B95 and MPWB1K Models and Comparative Assessments for Hydrogen Bonding and van der Waals Interactions. Journal of Physical Chemistry A, 2004, 108, 6908-6918.	1.1	1,497
10	Design of Density Functionals That Are Broadly Accurate for Thermochemistry, Thermochemical Kinetics, and Nonbonded Interactions. Journal of Physical Chemistry A, 2005, 109, 5656-5667.	1.1	1,451
11	Adiabatic Connection for Kinetics. Journal of Physical Chemistry A, 2000, 104, 4811-4815.	1.1	1,440
12	Density functional theory for transition metals and transition metal chemistry. Physical Chemistry Chemical Physics, 2009, 11, 10757.	1.3	1,431
13	Consistent van der Waals Radii for the Whole Main Group. Journal of Physical Chemistry A, 2009, 113, 5806-5812.	1.1	1,325
14	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
15	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. Journal of Chemical Theory and Computation, 2010, 6, 2872-2887.	2.3	1,183
16	Density Functional for Spectroscopy:Â No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States. Journal of Physical Chemistry A, 2006, 110, 13126-13130.	1.1	1,140
17	QM/MM: what have we learned, where are we, and where do we go from here?. Theoretical Chemistry Accounts, 2007, 117, 185-199.	0.5	1,053
18	How Enzymes Work: Analysis by Modern Rate Theory and Computer Simulations. Science, 2004, 303, 186-195.	6.0	1,048

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19	Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions. Journal of Chemical Physics, 2005, 123, 161103.	1.2	979
20	Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1849-1868.	2.3	956
21	Molecular modeling of the kinetic isotope effect for the [1,5]-sigmatropic rearrangement of cis-1,3-pentadiene. Journal of the American Chemical Society, 1993, 115, 2408-2415.	6.6	884
22	Variational transition-state theory. Accounts of Chemical Research, 1980, 13, 440-448.	7.6	874
23	Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. Journal of Physical Chemistry Letters, 2011, 2, 2810-2817.	2.1	864
24	MN15: A Kohnâ€“Sham global-hybrid exchangeâ€“correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. Chemical Science, 2016, 7, 5032-5051.	3.7	858
25	Aqueous Solvation Free Energies of Ions and Ionâ^'Water Clusters Based on an Accurate Value for the Absolute Aqueous Solvation Free Energy of the Proton. Journal of Physical Chemistry B, 2006, 110, 16066-16081.	1.2	856
26	Benchmark Databases for Nonbonded Interactions and Their Use To Test Density Functional Theory. Journal of Chemical Theory and Computation, 2005, 1, 415-432.	2.3	832
27	Parametrized Models of Aqueous Free Energies of Solvation Based on Pairwise Descreening of Solute Atomic Charges from a Dielectric Medium. The Journal of Physical Chemistry, 1996, 100, 19824-19839.	2.9	828
28	Use of Solution-Phase Vibrational Frequencies in Continuum Models for the Free Energy of Solvation. Journal of Physical Chemistry B, 2011, 115, 14556-14562.	1.2	828
29	Variational Transition State Theory. Annual Review of Physical Chemistry, 1984, 35, 159-189.	4.8	818
30	On the determination of Bornâ€“Oppenheimer nuclear motion wave functions including complications due to conical intersections and identical nuclei. Journal of Chemical Physics, 1979, 70, 2284-2296.	1.2	768
31	Current status of transition-state theory. The Journal of Physical Chemistry, 1983, 87, 2664-2682.	2.9	745
32	Benchmark Database of Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions and Its Use to Test Theoretical Methods. Journal of Physical Chemistry A, 2005, 109, 2012-2018.	1.1	736
33	QUANTUMMECHANICALMETHODS FORENZYMEKINETICS. Annual Review of Physical Chemistry, 2002, 53, 467-505.	4.8	730
34	Comparative DFT Study of van der Waals Complexes:Â Rare-Gas Dimers, Alkaline-Earth Dimers, Zinc Dimer, and Zinc-Rare-Gas Dimers. Journal of Physical Chemistry A, 2006, 110, 5121-5129.	1.1	706
35	Effectiveness of Diffuse Basis Functions for Calculating Relative Energies by Density Functional Theory. Journal of Physical Chemistry A, 2003, 107, 1384-1388.	1.1	688
36	Improved treatment of threshold contributions in variational transition-state theory. The Journal of Physical Chemistry, 1980, 84, 1730-1748.	2.9	678

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37	Conditions for the definition of a strictly diabatic electronic basis for molecular systems. Journal of Chemical Physics, 1982, 77, 6090-6098.	1.2	665
38	Applications and validations of the Minnesota density functionals. Chemical Physics Letters, 2011, 502, 1-13.	1.2	662
39	Charge Model 5: An Extension of Hirshfeld Population Analysis for the Accurate Description of Molecular Interactions in Gaseous and Condensed Phases. Journal of Chemical Theory and Computation, 2012, 8, 527-541.	2.3	661
40	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
41	Pairwise solute descreening of solute charges from a dielectric medium. Chemical Physics Letters, 1995, 246, 122-129.	1.2	648
42	Development and Assessment of a New Hybrid Density Functional Model for Thermochemical Kinetics. Journal of Physical Chemistry A, 2004, 108, 2715-2719.	1.1	639
43	Minimally augmented Karlsruhe basis sets. Theoretical Chemistry Accounts, 2011, 128, 295-305.	0.5	638
44	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120476.	1.6	599
45	Systematic study of basis set superposition errors in the calculated interaction energy of two HF molecules. Journal of Chemical Physics, 1985, 82, 2418-2426.	1.2	586
46	Basis-set extrapolation. Chemical Physics Letters, 1998, 294, 45-48.	1.2	580
47	Perspectives on Basis Sets Beautiful: Seasonal Plantings of Diffuse Basis Functions. Journal of Chemical Theory and Computation, 2011, 7, 3027-3034.	2.3	566
48	How Well Can Hybrid Density Functional Methods Predict Transition State Geometries and Barrier Heights?. Journal of Physical Chemistry A, 2001, 105, 2936-2941.	1.1	558
49	Functional representation of Liu and Siegbahnâ€™s accurate ab initio potential energy calculations for H+H2. Journal of Chemical Physics, 1978, 68, 2466-2476.	1.2	557
50	Density Functionals for Noncovalent Interaction Energies of Biological Importance. Journal of Chemical Theory and Computation, 2007, 3, 289-300.	2.3	557
51	A Universal Approach to Solvation Modeling. Accounts of Chemical Research, 2008, 41, 760-768.	7.6	536
52	POLYRATE 4: A new version of a computer program for the calculation of chemical reaction rates for polyatomics. Computer Physics Communications, 1992, 71, 235-262.	3.0	535
53	Modeling the Kinetics of Bimolecular Reactions. Chemical Reviews, 2006, 106, 4518-4584.	23.0	533
54	M11-L: A Local Density Functional That Provides Improved Accuracy for Electronic Structure Calculations in Chemistry and Physics. Journal of Physical Chemistry Letters, 2012, 3, 117-124.	2.1	531

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55	Screened-exchange density functionals with broad accuracy for chemistry and solid-state physics. Physical Chemistry Chemical Physics, 2012, 14, 16187.	1.3	525
56	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
57	Criterion of minimum state density in the transition state theory of bimolecular reactions. Journal of Chemical Physics, 1979, 70, 1593-1598.	1.2	495
58	Exact tunneling calculations. Journal of the American Chemical Society, 1971, 93, 1840-1851.	6.6	464
59	The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-821.	2.3	462
60	General parameterized SCF model for free energies of solvation in aqueous solution. Journal of the American Chemical Society, 1991, 113, 8305-8311.	6.6	457
61	Approximations for the exchange potential in electron scattering. Journal of Chemical Physics, 1975, 63, 2182-2191.	1.2	453
62	Single-Ion Solvation Free Energies and the Normal Hydrogen Electrode Potential in Methanol, Acetonitrile, and Dimethyl Sulfoxide. Journal of Physical Chemistry B, 2007, 111, 408-422.	1.2	452
63	Density Functionals for Inorganometallic and Organometallic Chemistry. Journal of Physical Chemistry A, 2005, 109, 11127-11143.	1.1	447
64	Abinitioeffective core potentials: Reduction of allâ€electron molecular structure calculations to calculations involving only valence electrons. Journal of Chemical Physics, 1976, 65, 3826-3853.	1.2	444
65	An SCF Solvation Model for the Hydrophobic Effect and Absolute Free Energies of Aqueous Solvation. Science, 1992, 256, 213-217.	6.0	439
66	Generalized transition state theory. Classical mechanical theory and applications to collinear reactions of hydrogen molecules. The Journal of Physical Chemistry, 1979, 83, 1052-1079.	2.9	430
67	Self-Consistent Reaction Field Model for Aqueous and Nonaqueous Solutions Based on Accurate Polarized Partial Charges. Journal of Chemical Theory and Computation, 2007, 3, 2011-2033.	2.3	426
68	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
69	Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-Molecule Solvation Free Energies. Journal of Physical Chemistry B, 2009, 113, 4538-4543.	1.2	418
70	SM6:Â A Density Functional Theory Continuum Solvation Model for Calculating Aqueous Solvation Free Energies of Neutrals, Ions, and Soluteâ^'Water Clusters. Journal of Chemical Theory and Computation, 2005, 1, 1133-1152.	2.3	414
71	Generalized transition state theory. Bond energy-bond order method for canonical variational calculations with application to hydrogen atom transfer reactions. Journal of the American Chemical Society, 1979, 101, 4534-4548.	6.6	409
72	Computational electrochemistry: prediction of liquid-phase reduction potentials. Physical Chemistry Chemical Physics, 2014, 16, 15068-15106.	1.3	407

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73	Adding Explicit Solvent Molecules to Continuum Solvent Calculations for the Calculation of Aqueous Acid Dissociation Constants. Journal of Physical Chemistry A, 2006, 110, 2493-2499.	1.1	405
74	Oxidation of ethane to ethanol by N2O in a metalâ€“organic framework with coordinatively unsaturated iron(II) sites. Nature Chemistry, 2014, 6, 590-595.	6.6	398
75	Multi-coefficient extrapolated density functional theory for thermochemistry and thermochemical kinetics. Physical Chemistry Chemical Physics, 2005, 7, 43.	1.3	393
76	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2010, 6, 2071-2085.	2.3	383
77	A double manyâ€body expansion of the two lowestâ€energy potential surfaces and nonadiabatic coupling for H3. Journal of Chemical Physics, 1987, 86, 6258-6269.	1.2	373
78	MN15-L: A New Local Exchange-Correlation Functional for Kohnâ€“Sham Density Functional Theory with Broad Accuracy for Atoms, Molecules, and Solids. Journal of Chemical Theory and Computation, 2016, 12, 1280-1293.	2.3	364
79	How Well Can New-Generation Density Functionals Describe the Energetics of Bond-Dissociation Reactions Producing Radicals?. Journal of Physical Chemistry A, 2008, 112, 1095-1099.	1.1	359
80	Model for Aqueous Solvation Based on Class IV Atomic Charges and First Solvation Shell Effects. The Journal of Physical Chemistry, 1996, 100, 16385-16398.	2.9	358
81	Mechanisms and Free Energies of Enzymatic Reactions. Chemical Reviews, 2006, 106, 3188-3209.	23.0	355
82	Symmetry numbers and chemical reaction rates. Theoretical Chemistry Accounts, 2007, 118, 813-826.	0.5	353
83	A simple approximation for the vibrational partition function of a hindered internal rotation. Journal of Computational Chemistry, 1991, 12, 266-270.	1.5	351
84	Direct dynamics calculation of the kinetic isotope effect for an organic hydrogen-transfer reaction, including corner-cutting tunneling in 21 dimensions. Journal of the American Chemical Society, 1993, 115, 7806-7817.	6.6	348
85	An improved and broadly accurate local approximation to the exchangeâ€“correlation density functional: The MN12-L functional for electronic structure calculations in chemistry and physics. Physical Chemistry Chemical Physics, 2012, 14, 13171.	1.3	346
86	Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 3669-3680.	2.3	334
87	Ab initio reaction paths and direct dynamics calculations. The Journal of Physical Chemistry, 1989, 93, 5107-5119.	2.9	329
88	Multidimensional Tunneling, Recrossing, and the Transmission Coefficient for Enzymatic Reactions. Chemical Reviews, 2006, 106, 3140-3169.	23.0	328
89	A general small-curvature approximation for transition-state-theory transmission coefficients. The Journal of Physical Chemistry, 1981, 85, 3019-3023.	2.9	321
90	AM1-SM2 and PM3-SM3 parameterized SCF solvation models for free energies in aqueous solution. Journal of Computer-Aided Molecular Design, 1992, 6, 629-666.	1.3	316

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91	Benchmark Energetic Data in a Model System for Grubbs II Metathesis Catalysis and Their Use for the Development, Assessment, and Validation of Electronic Structure Methods. Journal of Chemical Theory and Computation, 2009, 5, 324-333.	2.3	313
92	Cerium Metalâ€“Organic Framework for Photocatalysis. Journal of the American Chemical Society, 2018, 140, 7904-7912.	6.6	313
93	Class IV charge models: A new semiempirical approach in quantum chemistry. Journal of Computer-Aided Molecular Design, 1995, 9, 87-110.	1.3	309
94	The MIDI! basis set for quantum mechanical calculations of molecular geometries and partial charges. Theoretica Chimica Acta, 1996, 93, 281-301.	0.9	298
95	Doubly Hybrid Meta DFT:â€‰ New Multi-Coefficient Correlation and Density Functional Methods for Thermochemistry and Thermochemical Kinetics. Journal of Physical Chemistry A, 2004, 108, 4786-4791.	1.1	297
96	Interpolated variational transitionâ€state theory: Practical methods for estimating variational transitionâ€state properties and tunneling contributions to chemical reaction rates from electronic structure calculations. Journal of Chemical Physics, 1991, 95, 8875-8894.	1.2	296
97	Small Representative Benchmarks for Thermochemical Calculations. Journal of Physical Chemistry A, 2003, 107, 8996-8999.	1.1	288
98	Coherent switching with decay of mixing: An improved treatment of electronic coherence for non-Bornâ€“Oppenheimer trajectories. Journal of Chemical Physics, 2004, 121, 7658.	1.2	288
99	Reactive Scattering Cross Sections III: Quasiclassical and Semiclassical Methods. , 1979, , 505-566.		288
100	Direct dynamics calculations with NDDO (neglect of diatomic differential overlap) molecular orbital theory with specific reaction parameters. The Journal of Physical Chemistry, 1991, 95, 4618-4627.	2.9	285
101	From Force Fields to Dynamics: Classical and Quantal Paths. Science, 1990, 249, 491-498.	6.0	284
102	Aqueous Mg-Ion Battery Based on Polyimide Anode and Prussian Blue Cathode. ACS Energy Letters, 2017, 2, 1115-1121.	8.8	283
103	Variational transition state theory: theoretical framework and recent developments. Chemical Society Reviews, 2017, 46, 7548-7596.	18.7	281
104	Statistical thermodynamics of bond torsional modes. Journal of Chemical Physics, 2000, 112, 1221-1228.	1.2	276
105	Exchangeâ€“Correlation Functional with Good Accuracy for Both Structural and Energetic Properties while Depending Only on the Density and Its Gradient. Journal of Chemical Theory and Computation, 2012, 8, 2310-2319.	2.3	276
106	Variational Transition State Theory with Multidimensional Tunneling. Reviews in Computational Chemistry, 2007, , 125-232.	1.5	273
107	Polyatomic canonical variational theory for chemical reaction rates. Separableâ€mode formalism with application to OH+H2â†'H2O+H. Journal of Chemical Physics, 1982, 76, 1380-1391.	1.2	268
108	Atmospheric Chemistry of Criegee Intermediates: Unimolecular Reactions and Reactions with Water. Journal of the American Chemical Society, 2016, 138, 14409-14422.	6.6	265

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109	Construction of a generalized gradient approximation by restoring the density-gradient expansion and enforcing a tight Liebâ€“Oxford bound. Journal of Chemical Physics, 2008, 128, 184109.	1.2	260
110	New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. Journal of Physical Chemistry A, 1998, 102, 1820-1831.	1.1	259
111	Mapped Interpolation Scheme for Single-Point Energy Corrections in Reaction Rate Calculations and a Critical Evaluation of Dual-Level Reaction Path Dynamics Methods. Journal of Physical Chemistry A, 1999, 103, 1140-1149.	1.1	254
112	Electrostatically Embedded Many-Body Expansion for Large Systems, with Applications to Water Clusters. Journal of Chemical Theory and Computation, 2007, 3, 46-53.	2.3	254
113	Communication: A global hybrid generalized gradient approximation to the exchange-correlation functional that satisfies the second-order density-gradient constraint and has broad applicability in chemistry. Journal of Chemical Physics, 2011, 135, 191102.	1.2	254
114	Robust and Affordable Multicoefficient Methods for Thermochemistry and Thermochemical Kinetics:â€‰ The MCCM/3 Suite and SAC/3. Journal of Physical Chemistry A, 2003, 107, 3898-3906.	1.1	252
115	Vibrationally adiabatic models for reactive tunneling. Journal of Chemical Physics, 1982, 77, 5955-5976.	1.2	250
116	Quasifree-scattering model for the imaginary part of the optical potential for electron scattering. Physical Review A, 1983, 28, 2740-2751.	1.0	247
117	How well can new-generation density functional methods describe stacking interactions in biological systems?. Physical Chemistry Chemical Physics, 2005, 7, 2701.	1.3	246
118	Semiclassical tunneling calculations. The Journal of Physical Chemistry, 1979, 83, 2921-2926.	2.9	245
119	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3832-3839.	2.3	245
120	Factors Affecting Competitive Ionâˆ’Molecule Reactions:â€‰ ClO- + C2H5Cl and C2D5Cl via E2 and SN2 Channels. Journal of the American Chemical Society, 1996, 118, 860-869.	6.6	243
121	Perspective: Kohn-Sham density functional theory descending a staircase. Journal of Chemical Physics, 2016, 145, 130901.	1.2	243
122	Variational transition state theory and tunneling for a heavyâ€“lightâ€“heavy reaction using an ab initio potential energy surface. 37Cl+H(D) 35Clâ†’H(D) 37Cl+35Cl. Journal of Chemical Physics, 1983, 78, 4400-4413.	1.2	242
123	Tests of second-generation and third-generation density functionals for thermochemical kineticsElectronic supplementary information (ESI) available: Mean errors for pure and hybrid DFT methods. See http://www.rsc.org/suppdata/cp/b3/b316260e/. Physical Chemistry Chemical Physics, 2004, 6, 673.	1.3	242
124	Quantum-Chemical Characterization of the Properties and Reactivities of Metalâ€“Organic Frameworks. Chemical Reviews, 2015, 115, 6051-6111.	23.0	241
125	The Incorporation of Quantum Effects in Enzyme Kinetics Modeling. Accounts of Chemical Research, 2002, 35, 341-349.	7.6	240
126	Efficient Diffuse Basis Sets: cc-pVxZ+ and maug-cc-pVxZ. Journal of Chemical Theory and Computation, 2009, 5, 1197-1202.	2.3	236

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127	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. Accounts of Chemical Research, 2017, 50, 66-73.	7.6	232
128	Ab initio transition state theory calculations of the reaction rate for OH+CH4â†'H2O+CH3. Journal of Chemical Physics, 1990, 93, 1761-1769.	1.2	228
129	Quantum Mechanical Continuum Solvation Models for Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 9122-9129.	1.2	225
130	Generalized transition state theory. Quantum effects for collinear reactions of hydrogen molecules and isotopically substituted hydrogen molecules. The Journal of Physical Chemistry, 1979, 83, 1079-1112.	2.9	223
131	Exact and Approximate Quantum Mechanical Reaction Probabilities and Rate Constants for the Collinear H + H2Reaction. Journal of Chemical Physics, 1972, 56, 2232-2252.	1.2	221
132	History of H3 Kinetics. Annual Review of Physical Chemistry, 1976, 27, 1-43.	4.8	221
133	Incorporation of quantum effects in generalized-transition-state theory. The Journal of Physical Chemistry, 1982, 86, 2252-2261.	2.9	220
134	Computational characterization and modeling of buckyball tweezers: density functional study of concaveâ€"convex Ï€â‹¯Ï€ interactions. Physical Chemistry Chemical Physics, 2008, 10, 2813.	1.3	218
135	A leastâ€action variational method for calculating multidimensional tunneling probabilities for chemical reactions. Journal of Chemical Physics, 1983, 79, 4931-4938.	1.2	216
136	Status and Challenges of Density Functional Theory. Trends in Chemistry, 2020, 2, 302-318.	4.4	216
137	Assessment of Model Chemistries for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2006, 2, 1009-1018.	2.3	214
138	Chemical Kinetics and Mechanisms of Complex Systems: AÂPerspective on Recent Theoretical Advances. Journal of the American Chemical Society, 2014, 136, 528-546.	6.6	212
139	Databases for Transition Element Bonding:Â Metalâ^'Metal Bond Energies and Bond Lengths and Their Use To Test Hybrid, Hybrid Meta, and Meta Density Functionals and Generalized Gradient Approximations. Journal of Physical Chemistry A, 2005, 109, 4388-4403.	1.1	209
140	Performance of the M06 family of exchange-correlation functionals for predicting magnetic coupling in organic and inorganic molecules. Journal of Chemical Physics, 2008, 128, 114103.	1.2	208
141	Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. Journal of Chemical Theory and Computation, 2007, 3, 569-582.	2.3	207
142	Computation of equilibrium oxidation and reduction potentials for reversible and dissociative electron-transfer reactions in solution. Theoretical Chemistry Accounts, 2004, 112, 217.	0.5	206
143	Tests of the RPBE, revPBE, Ï„-HCTHhyb, Ï‰B97X-D, and MOHLYP density functional approximations and 29 others against representative databases for diverse bond energies and barrier heights in catalysis. Journal of Chemical Physics, 2010, 132, 164117.	1.2	206
144	Reactionâ€path potential and vibrational frequencies in terms of curvilinear internal coordinates. Journal of Chemical Physics, 1995, 102, 3188-3201.	1.2	202

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145	Reaction-Path Energetics and Kinetics of the Hydride Transfer Reaction Catalyzed by Dihydrofolate Reductase. Biochemistry, 2003, 42, 13558-13575.	1.2	202
146	Practical computation of electronic excitation in solution: vertical excitation model. Chemical Science, 2011, 2, 2143.	3.7	202
147	Convergent Partially Augmented Basis Sets for Post-Hartreeâ^'Fock Calculations of Molecular Properties and Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2011, 7, 10-18.	2.3	201
148	Multi-coefficient Gaussian-3 method for calculating potential energy surfaces. Chemical Physics Letters, 1999, 306, 407-410.	1.2	198
149	Extension of the platform of applicability of the SM5.42R universal solvation model. Theoretical Chemistry Accounts, 1999, 103, 9-63.	0.5	197
150	Non-Bornâ^'Oppenheimer Molecular Dynamics. Accounts of Chemical Research, 2006, 39, 101-108.	7.6	197
151	Parabolic tunneling calculations. The Journal of Physical Chemistry, 1981, 85, 624-628.	2.9	196
152	Assessment of Density Functionals for Ï€ Systems:Â Energy Differences between Cumulenes and Poly-ynes; Proton Affinities, Bond Length Alternation, and Torsional Potentials of Conjugated Polyenes; and Proton Affinities of Conjugated Shiff Bases. Journal of Physical Chemistry A, 2006, 110, 10478-10486.	1.1	196
153	Practical methods for including torsional anharmonicity in thermochemical calculations on complex molecules: The internal-coordinate multi-structural approximation. Physical Chemistry Chemical Physics, 2011, 13, 10885.	1.3	196
154	Computational electrochemistry: aqueous one-electron oxidation potentials for substituted anilines. Physical Chemistry Chemical Physics, 2000, 2, 1231-1239.	1.3	194
155	Carbon Tunneling from a Single Quantum State. Science, 2003, 299, 867-870.	6.0	194
156	Investigation of the shape of the imaginary part of the optical-model potential for electron scattering by rare gases. Physical Review A, 1984, 29, 3078-3091.	1.0	193
157	A Density Functional That Accounts for Medium-Range Correlation Energies in Organic Chemistry. Organic Letters, 2006, 8, 5753-5755.	2.4	193
158	Trajectoryâ€surfaceâ€hopping study of Na(3pâ€‰2P) +H2â€‰â†'â€‰Na(3sâ€‰2S)+H2(vâ€²,â€‰jâ€²,â€‰Î). Journal of Chemical 1334-1342.	1.2	192
159	Introductory lecture: Nonadiabatic effects in chemical dynamics. Faraday Discussions, 2004, 127, 1.	1.6	190
160	Density Functional Theory for Reaction Energies: Test of Meta and Hybrid Meta Functionals, Range-Separated Functionals, and Other High-Performance Functionals. Journal of Chemical Theory and Computation, 2011, 7, 669-676.	2.3	190
161	Potential energy surfaces for polyatomic reaction dynamics. Chemical Reviews, 1987, 87, 217-236.	23.0	187
162	Algorithms and accuracy requirements for computing reaction paths by the method of steepest descent. The Journal of Physical Chemistry, 1988, 92, 1476-1488.	2.9	187

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163	The direct calculation of diabatic states based on configurational uniformity. Journal of Chemical Physics, 2001, 115, 10353.	1.2	187
164	Quantum chemical conformational analysis of glucose in aqueous solution. Journal of the American Chemical Society, 1993, 115, 5745-5753.	6.6	185
165	Relative stability of alternative chair forms and hydroxymethyl conformations of Î²-d-glucopyranose. Carbohydrate Research, 1995, 276, 219-251.	1.1	184
166	Optimized Parameters for Scaling Correlation Energy. Journal of Physical Chemistry A, 1999, 103, 3139-3143.	1.1	184
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