Martin Head-Gordon

List of Publications by Year
in descending order

425 papers	69,605 citations	2544 96 h-index	677 254 g-index
445 all docs	445 docs citations	445 times ranked	36177 citing authors

#	Article	IF	Citations
1	Long-range corrected hybrid density functionals with damped atomâ€“atom dispersion corrections. Physical Chemistry Chemical Physics, 2008, 10, 6615.	2.8	10,464
2	A fifth-order perturbation comparison of electron correlation theories. Chemical Physics Letters, 1989, 157, 479-483.	2.6	7,448
3	Systematic optimization of long-range corrected hybrid density functionals. Journal of Chemical Physics, 2008, 128, 084106.	3.0	2,890
4	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
5	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
6	Single-Reference ab Initio Methods for the Calculation of Excited States of Large Molecules. Chemical Reviews, 2005, 105, 4009-4037.	47.7	2,315
7	Toward a systematic molecular orbital theory for excited states. The Journal of Physical Chemistry, 1992, 96, 135-149.	2.9	2,277
8	Time-dependent density functional theory within the Tammâ€“Dancoff approximation. Chemical Physics Letters, 1999, 314, 291-299.	2.6	1,724
9	Failure of Time-Dependent Density Functional Theory for Long-Range Charge-Transfer Excited States:Â The Zincbacteriochlorinâ^'Bacteriochlorin and Bacteriochlorophyllâ^'Spheroidene Complexes. Journal of the American Chemical Society, 2004, 126, 4007-4016.	13.7	1,561
10	Long-range charge-transfer excited states in time-dependent density functional theory require non-local exchange. Journal of Chemical Physics, 2003, 119, 2943-2946.	3.0	1,416
11	Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. Molecular Physics, 2017, 115, 2315-2372.	1.7	1,401
12	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	2.6	1,093
13	Simulated Quantum Computation of Molecular Energies. Science, 2005, 309, 1704-1707.	12.6	852
14	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	3.3	617
15	Ï‰B97X-V: A 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. Physical Chemistry Chemical Physics, 2014, 16, 9904.	2.8	616
16	A doubles correction to electronic excited states from configuration interaction in the space of single substitutions. Chemical Physics Letters, 1994, 219, 21-29.	2.6	610
17	Mechanism of CO₂ Reduction at Copper Surfaces: Pathways to C₂ Products. ACS Catalysis, 2018, 8, 1490-1499.	11.2	608
18	Ï‰B97M-V: A combinatorially optimized, range-separated hybrid, meta-GGA density functional with VV10 nonlocal correlation. Journal of Chemical Physics, 2016, 144, 214110.	3.0	595

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19	The spinâ€“flip approach within time-dependent density functional theory: Theory and applications to diradicals. Journal of Chemical Physics, 2003, 118, 4807-4818.	3.0	581
20	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
21	Unravelling the Origin of Intermolecular Interactions Using Absolutely Localized Molecular Orbitals. Journal of Physical Chemistry A, 2007, 111, 8753-8765.	2.5	508
22	Scaled opposite-spin second order MÃ¸llerâ€“Plesset correlation energy: An economical electronic structure method. Journal of Chemical Physics, 2004, 121, 9793-9802.	3.0	492
23	Identification of Possible Pathways for Câ€“C Bond Formation during Electrochemical Reduction of CO₂: New Theoretical Insights from an Improved Electrochemical Model. Journal of Physical Chemistry Letters, 2016, 7, 1471-1477.	4.6	479
24	Size-consistent Brueckner theory limited to double substitutions. Chemical Physics Letters, 1989, 164, 185-192.	2.6	478
25	Resonance-stabilized hydrocarbon-radical chain reactions may explain soot inception and growth. Science, 2018, 361, 997-1000.	12.6	472
26	Highly correlated calculations with a polynomial cost algorithm: A study of the density matrix renormalization group. Journal of Chemical Physics, 2002, 116, 4462-4476.	3.0	459
27	The continuous fast multipole method. Chemical Physics Letters, 1994, 230, 8-16.	2.6	370
28	How Accurate Are the Minnesota Density Functionals for Noncovalent Interactions, Isomerization Energies, Thermochemistry, and Barrier Heights Involving Molecules Composed of Main-Group Elements?. Journal of Chemical Theory and Computation, 2016, 12, 4303-4325.	5.3	355
29	Linear scaling density functional calculations via the continuous fast multipole method. Chemical Physics Letters, 1996, 253, 268-278.	2.6	327
30	Long-range corrected double-hybrid density functionals. Journal of Chemical Physics, 2009, 131, 174105.	3.0	327
31	Fifth order Moeller-Plesset perturbation theory: comparison of existing correlation methods and implementation of new methods correct to fifth order. The Journal of Physical Chemistry, 1990, 94, 5579-5586.	2.9	305
32	Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V. Journal of Chemical Physics, 2015, 142, 074111.	3.0	305
33	Linear and sublinear scaling formation of Hartreeâ€“Fock-type exchange matrices. Journal of Chemical Physics, 1998, 109, 1663-1669.	3.0	302
34	Analysis of Electronic Transitions as the Difference of Electron Attachment and Detachment Densities. The Journal of Physical Chemistry, 1995, 99, 14261-14270.	2.9	288
35	Intermolecular Ï€-to-Ï€ Bonding between Stacked Aromatic Dyads. Experimental and Theoretical Binding Energies and Near-IR Optical Transitions for Phenalenyl Radical/Radical versus Radical/Cation Dimerizations. Journal of the American Chemical Society, 2004, 126, 13850-13858.	13.7	286
36	Characterizing unpaired electrons from the one-particle density matrix. Chemical Physics Letters, 2003, 372, 508-511.	2.6	274

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37	Probing non-covalent interactions with a second generation energy decomposition analysis using absolutely localized molecular orbitals. Physical Chemistry Chemical Physics, 2016, 18, 23067-23079.	2.8	264
38	Generalized Unitary Coupled Cluster Wave functions for Quantum Computation. Journal of Chemical Theory and Computation, 2019, 15, 311-324.	5.3	260
39	Quantum Chemistry and Molecular Processes. The Journal of Physical Chemistry, 1996, 100, 13213-13225.	2.9	232
40	Energies and analytic gradients for a coupled-cluster doubles model using variational Brueckner orbitals: Application to symmetry breaking in O4+. Journal of Chemical Physics, 1998, 109, 4171-4181.	3.0	228
41	Optimized spin-component scaled second-order MÃ¸ller-Plesset perturbation theory for intermolecular interaction energies. Molecular Physics, 2007, 105, 1073-1083.	1.7	225
42	Dispersion-corrected MÃ¸llerâ€“Plesset second-order perturbation theory. Journal of Chemical Physics, 2009, 131, 094106.	3.0	223
43	Size-consistent wave functions for nondynamical correlation energy: The valence active space optimized orbital coupled-cluster doubles model. Journal of Chemical Physics, 1998, 109, 10669-10678.	3.0	222
44	Mechanistic insights into electrochemical reduction of CO ₂ over Ag using density functional theory and transport models. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E8812-E8821.	7.1	219
45	A deterministic alternative to the full configuration interaction quantum Monte Carlo method. Journal of Chemical Physics, 2016, 145, 044112.	3.0	218
46	Time-dependent density functional study on the electronic excitation energies of polycyclic aromatic hydrocarbon radical cations of naphthalene, anthracene, pyrene, and perylene. Journal of Chemical Physics, 1999, 111, 8904-8912.	3.0	208
47	M₂(m-dobdc) (M = Mg, Mn, Fe, Co, Ni) Metalâ€“Organic Frameworks Exhibiting Increased Charge Density and Enhanced H₂ Binding at the Open Metal Sites. Journal of the American Chemical Society, 2014, 136, 12119-12129.	13.7	207
48	Restricted active space spin-flip configuration interaction approach: theory, implementation and examples. Physical Chemistry Chemical Physics, 2009, 11, 9779.	2.8	202
49	Linear scaling computation of the Fock matrix. II. Rigorous bounds on exchange integrals and incremental Fock build. Journal of Chemical Physics, 1997, 106, 9708-9717.	3.0	195
50	Analysis of charge transfer effects in molecular complexes based on absolutely localized molecular orbitals. Journal of Chemical Physics, 2008, 128, 184112.	3.0	188
51	Vibronically coherent ultrafast triplet-pair formation and subsequent thermally activated dissociation control efficient endothermic singlet fission. Nature Chemistry, 2017, 9, 1205-1212.	13.6	184
52	Configuration interaction singles, time-dependent Hartreeâ€“Fock, and time-dependent density functional theory for the electronic excited states of extended systems. Journal of Chemical Physics, 1999, 111, 10774-10786.	3.0	181
53	How Accurate Is Density Functional Theory at Predicting Dipole Moments? An Assessment Using a New Database of 200 Benchmark Values. Journal of Chemical Theory and Computation, 2018, 14, 1969-1981.	5.3	180
54	An efficient self-consistent field method for large systems of weakly interacting components. Journal of Chemical Physics, 2006, 124, 204105.	3.0	179

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55	Closely approximating second-order Mo/llerâ€“Plesset perturbation theory with a local triatomics in molecules model. Journal of Chemical Physics, 2000, 112, 3592-3601.	3.0	173
56	Catalytic proton reduction with transition metal complexes of the redox-active ligand bpy2PYMe. Chemical Science, 2013, 4, 3934.	7.4	166
57	An assessment of strategies for the development of solid-state adsorbents for vehicular hydrogen storage. Energy and Environmental Science, 2018, 11, 2784-2812.	30.8	162
58	A perturbative correction to restricted open shell configuration interaction with single substitutions for excited states of radicals. Chemical Physics Letters, 1995, 246, 114-121.	2.6	158
59	Second-order perturbation corrections to singles and doubles coupled-cluster methods: General theory and application to the valence optimized doubles model. Journal of Chemical Physics, 2000, 113, 3548-3560.	3.0	155
60	A second-order perturbative correction to the coupled-cluster singles and doubles method: CCSD(2). Journal of Chemical Physics, 2001, 115, 2014-2021.	3.0	154
61	Efficient exploration of reaction paths via a freezing string method. Journal of Chemical Physics, 2011, 135, 224108.	3.0	154
62	Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. ACS Catalysis, 2019, 9, 920-931.	11.2	153
63	Electronic Absorption Spectra of Neutral Perylene (C20H12), Terrylene (C30H16), and Quaterrylene (C40H20) and Their Positive and Negative Ions:â€‰ Ne Matrix-Isolation Spectroscopy and Time-Dependent Density Functional Theory Calculations. Journal of Physical Chemistry A, 2003, 107, 3660-3669.	2.5	151
64	A Correlated Electron View of Singlet Fission. Accounts of Chemical Research, 2013, 46, 1339-1347.	15.6	150
65	Orbital-optimized opposite-spin scaled second-order correlation: An economical method to improve the description of open-shell molecules. Journal of Chemical Physics, 2007, 126, 164101.	3.0	148
66	Analysis of the Reaction Mechanism and Catalytic Activity of Metal-Substituted Beta Zeolite for the Isomerization of Glucose to Fructose. ACS Catalysis, 2014, 4, 1537-1545.	11.2	148
67	A tensor formulation of many-electron theory in a nonorthogonal single-particle basis. Journal of Chemical Physics, 1998, 108, 616-625.	3.0	145
68	The Theoretical Prediction of Molecular Radical Species:â€‰ a Systematic Study of Equilibrium Geometries and Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2001, 105, 9736-9747.	2.5	142
69	Linear scaling density fitting. Journal of Chemical Physics, 2006, 125, 194109.	3.0	141
70	Impact of Metal and Anion Substitutions on the Hydrogen Storage Properties of M-BTT Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2013, 135, 1083-1091.	13.7	139
71	Characterizing the interplay of Pauli repulsion, electrostatics, dispersion and charge transfer in halogen bonding with energy decomposition analysis. Physical Chemistry Chemical Physics, 2018, 20, 905-915.	2.8	139
72	A second-order correction to singles and doubles coupled-cluster methods based on a perturbative expansion of a similarity-transformed Hamiltonian. Chemical Physics Letters, 2000, 323, 21-28.	2.6	137

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73	A geometric approach to direct minimization. Molecular Physics, 2002, 100, 1713-1721.	1.7	137
74	Charge-Transfer State as a Possible Signature of a Zeaxanthinâ^'Chlorophyll Dimer in the Non-photochemical Quenching Process in Green Plants. Journal of Physical Chemistry B, 2003, 107, 6500-6503.	2.6	136
75	Survival of the most transferable at the top of Jacobâ€™s ladder: Defining and testing the Ï‰B97M(2) double hybrid density functional. Journal of Chemical Physics, 2018, 148, 241736.	3.0	136
76	Electron Donation in the Waterâ€“Water Hydrogen Bond. Chemistry - A European Journal, 2009, 15, 851-855.	3.3	135
77	An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order MÃ¸ller-Plesset perturbation theory: Application to alanine tetrapeptide conformational analysis. Journal of Computational Chemistry, 2007, 28, 839-856.	3.3	134
78	LOBA: a localized orbital bonding analysis to calculate oxidation states, with application to a model water oxidation catalyst. Physical Chemistry Chemical Physics, 2009, 11, 11297.	2.8	134
79	Efficient evaluation of the Coulomb force in density-functional theory calculations. Journal of Chemical Physics, 2001, 114, 6572-6577.	3.0	132
80	On the performance of density functional theory for symmetry-breaking problems. Chemical Physics Letters, 1999, 302, 425-430.	2.6	128
81	Defining the contributions of permanent electrostatics, Pauli repulsion, and dispersion in density functional theory calculations of intermolecular interaction energies. Journal of Chemical Physics, 2016, 144, 114107.	3.0	127
82	Excited states theory for optimized orbitals and valence optimized orbitals coupled-cluster doubles models. Journal of Chemical Physics, 2000, 113, 6509-6527.	3.0	125
83	Chlorophyll fluorescence quenching by xanthophylls. Physical Chemistry Chemical Physics, 2003, 5, 3247.	2.8	120
84	Is Subsurface Oxygen Necessary for the Electrochemical Reduction of CO₂ on Copper?. Journal of Physical Chemistry Letters, 2018, 9, 601-606.	4.6	118
85	Benchmark variational coupled cluster doubles results. Journal of Chemical Physics, 2000, 113, 8873-8879.	3.0	114
86	Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2014, 141, 024102.	3.0	113
87	A coupled-cluster ab initio study of triplet C3H2 and the neutralâ€“neutral reaction to interstellar C3H. Journal of Chemical Physics, 1997, 106, 4141-4151.	3.0	110
88	Improved Force-Field Parameters for QM/MM Simulations of the Energies of Adsorption for Molecules in Zeolites and a Free Rotor Correction to the Rigid Rotor Harmonic Oscillator Model for Adsorption Enthalpies. Journal of Physical Chemistry C, 2015, 119, 1840-1850.	3.1	110
89	Exact solution (within a triple-zeta, double polarization basis set) of the electronic SchrÃ¶dinger equation for water. Journal of Chemical Physics, 2003, 118, 8551-8554.	3.0	109
90	Charged polycyclic aromatic hydrocarbon clusters and the galactic extended red emission. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 5274-5278.	7.1	109

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91	How Diradicaloid Is a Stable Diradical?. ChemPhysChem, 2003, 4, 522-525.	2.1	107
92	Mechanism and Kinetics of Propane Dehydrogenation and Cracking over Ga/H-MFI Prepared via Vapor-Phase Exchange of H-MFI with GaCl‹sub›3‹/sub›. Journal of the American Chemical Society, 2019, 141, 1614-1627.	13.7	107
93	Excited State Orbital Optimization via Minimizing the Square of the Gradient: General Approach and Application to Singly and Doubly Excited States via Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 1699-1710.	5.3	106
94	Mechanism of the Electrocatalytic Reduction of Protons with Diaryldithiolene Cobalt Complexes. Journal of the American Chemical Society, 2014, 136, 9364-9376.	13.7	102
95	Bioinspired design of redox-active ligands for multielectron catalysis: effects of positioning pyrazine reservoirs on cobalt for electro- and photocatalytic generation of hydrogen from water. Chemical Science, 2015, 6, 4954-4972.	7.4	99
96	Self-interaction error of local density functionals for alkaliâ€“halide dissociation. Chemical Physics Letters, 2006, 422, 230-233.	2.6	98
97	Time-Dependent Density Functional Study of the Electronic Excited States of Polycyclic Aromatic Hydrocarbon Radical Ions. Journal of Physical Chemistry A, 2003, 107, 4940-4951.	2.5	96
98	Ab initio molecular dynamics simulations of liquid water using high quality meta-GGA functionals. Chemical Science, 2017, 8, 3554-3565.	7.4	95
99	How accurate are static polarizability predictions from density functional theory? An assessment over 132 species at equilibrium geometry. Physical Chemistry Chemical Physics, 2018, 20, 19800-19810.	2.8	94
100	Orbital Optimized Density Functional Theory for Electronic Excited States. Journal of Physical Chemistry Letters, 2021, 12, 4517-4529.	4.6	92
101	Polarization contributions to intermolecular interactions revisited with fragment electric-field response functions. Journal of Chemical Physics, 2015, 143, 114111.	3.0	91
102	Characterizing the Dimerizations of Phenalenyl Radicals by ab Initio Calculations and Spectroscopy:â€‰ Ïƒ-Bond Formation versus Resonance Ï€-Stabilization. Journal of Physical Chemistry A, 2005, 109, 11261-11267.	2.5	90
103	A Resolution-Of-The-Identity Implementation of the Local Triatomics-In-Molecules Model for Second-Order MÃ¸llerâ€“Plesset Perturbation Theory with Application to Alanine Tetrapeptide Conformational Energies. Journal of Chemical Theory and Computation, 2005, 1, 862-876.	5.3	90
104	Hartreeâ€“Fock solutions as a quasidiabatic basis for nonorthogonal configuration interaction. Journal of Chemical Physics, 2009, 131, 124113.	3.0	90
105	Unrestricted absolutely localized molecular orbitals for energy decomposition analysis: Theory and applications to intermolecular interactions involving radicals. Journal of Chemical Physics, 2013, 138, 134119.	3.0	90
106	Beyond Energies: Geometries of Nonbonded Molecular Complexes as Metrics for Assessing Electronic Structure Approaches. Journal of Chemical Theory and Computation, 2015, 11, 1481-1492.	5.3	90
107	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
108	Modern Approaches to Exact Diagonalization and Selected Configuration Interaction with the Adaptive Sampling CI Method. Journal of Chemical Theory and Computation, 2020, 16, 2139-2159.	5.3	90

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109	Computational Modeling of the Nature and Role of Ga Species for Light Alkane Dehydrogenation Catalyzed by Ga/H-MFI. ACS Catalysis, 2018, 8, 6146-6162.	11.2	86
110	Improved Fermi operator expansion methods for fast electronic structure calculations. Journal of Chemical Physics, 2003, 119, 4117-4125.	3.0	85
111	Energy decomposition analysis of single bonds within Kohnâ€“Sham density functional theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 12649-12656.	7.1	85
112	Characterization of Isolated Ga³⁺ Cations in Ga/H-MFI Prepared by Vapor-Phase Exchange of H-MFI Zeolite with GaCl₃. ACS Catalysis, 2018, 8, 6106-6126.	11.2	85
113	CASSCF with Extremely Large Active Spaces Using the Adaptive Sampling Configuration Interaction Method. Journal of Chemical Theory and Computation, 2020, 16, 2340-2354.	5.3	85
114	What is the nature of the long bond in the TCNE22â^Ï€-dimer?. Physical Chemistry Chemical Physics, 2004, 6, 2008-2011.	2.8	83
115	Scaled Opposite Spin Second Order MÃ¸llerâ^'Plesset Theory with Improved Physical Description of Long-Range Dispersion Interactions. Journal of Physical Chemistry A, 2005, 109, 7598-7605.	2.5	83
116	Benchmark results for empirical post-GGA functionals: Difficult exchange problems and independent tests. Physical Chemistry Chemical Physics, 2011, 13, 19325.	2.8	83
117	Characterizing and Understanding the Remarkably Slow Basis Set Convergence of Several Minnesota Density Functionals for Intermolecular Interaction Energies. Journal of Chemical Theory and Computation, 2013, 9, 4453-4461.	5.3	83
118	Highly Accurate Prediction of Core Spectra of Molecules at Density Functional Theory Cost: Attaining Sub-electronvolt Error from a Restricted Open-Shell Kohnâ€“Sham Approach. Journal of Physical Chemistry Letters, 2020, 11, 775-786.	4.6	82
119	Fast localized orthonormal virtual orbitals which depend smoothly on nuclear coordinates. Journal of Chemical Physics, 2005, 123, 114108.	3.0	81
120	Ambient-Temperature Hydrogen Storage via Vanadium(II)-Dihydrogen Complexation in a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2021, 143, 6248-6256.	13.7	81
121	Hydrogen Physisorption on Metalâ€“Organic Framework Linkers and Metalated Linkers: A Computational Study of the Factors That Control Binding Strength. Journal of the American Chemical Society, 2014, 136, 17827-17835.	13.7	80
122	A perturbative correction to the quadratic coupled-cluster doubles method for higher excitations. Chemical Physics Letters, 2002, 353, 359-367.	2.6	79
123	Tailoring Metal-Porphyrin-Like Active Sites on Graphene to Improve the Efficiency and Selectivity of Electrochemical CO₂ Reduction. Journal of Physical Chemistry C, 2015, 119, 21345-21352.	3.1	79
124	Assessing Ionâ€“Water Interactions in the AMOEBA Force Field Using Energy Decomposition Analysis of Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2016, 12, 5422-5437.	5.3	79
125	Regularized Orbital-Optimized Second-Order MÃ¸llerâ€“Plesset Perturbation Theory: A Reliable Fifth-Order-Scaling Electron Correlation Model with Orbital Energy Dependent Regularizers. Journal of Chemical Theory and Computation, 2018, 14, 5203-5219.	5.3	79
126	Use of the rVV10 Nonlocal Correlation Functional in the B97M-V Density Functional: Defining B97M-rV and Related Functionals. Journal of Physical Chemistry Letters, 2017, 8, 35-40.	4.6	78

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127	Simulations of femtosecond laser-induced desorption of CO from Cu(100). Surface Science, 1994, 320, L57-L62.	1.9	77
128	Advanced Potential Energy Surfaces for Molecular Simulation. Journal of Physical Chemistry B, 2016, 120, 9811-9832.	2.6	77
129	Metalâ€“Ligand Cooperativity via Exchange Coupling Promotes Iron- Catalyzed Electrochemical CO₂ Reduction at Low Overpotentials. Journal of the American Chemical Society, 2020, 142, 20489-20501.	13.7	77
130	Approaching the Basis Set Limit in Density Functional Theory Calculations Using Dual Basis Sets without Diagonalizationâ€. Journal of Physical Chemistry A, 2004, 108, 3206-3210.	2.5	76
131	Periodic boundary conditions and the fast multipole method. Journal of Chemical Physics, 1997, 107, 10131-10140.	3.0	75
132	Locating Multiple Self-Consistent Field Solutions: An Approach Inspired by Metadynamics. Physical Review Letters, 2008, 101, 193001.	7.8	74
133	On the Nature of Electronic Transitions in Radicals:â€‰ An Extended Single Excitation Configuration Interaction Method. The Journal of Physical Chemistry, 1996, 100, 6131-6137.	2.9	71
134	The quadratic coupled cluster doubles model. Chemical Physics Letters, 2000, 330, 585-594.	2.6	71
135	Assessing DFT-D3 Damping Functions Across Widely Used Density Functionals: Can We Do Better?. Journal of Chemical Theory and Computation, 2017, 13, 2043-2052.	5.3	71
136	Delocalization Errors in Density Functional Theory Are Essentially Quadratic in Fractional Occupation Number. Journal of Physical Chemistry Letters, 2018, 9, 6280-6288.	4.6	71
137	An energy decomposition analysis for intermolecular interactions from an absolutely localized molecular orbital reference at the coupled-cluster singles and doubles level. Journal of Chemical Physics, 2012, 136, 024103.	3.0	70
138	Restricted active space spin-flip configuration interaction: Theory and examples for multiple spin flips with odd numbers of electrons. Journal of Chemical Physics, 2012, 137, 164110.	3.0	69
139	The Performance of Density Functionals for Sulfateâ€“Water Clusters. Journal of Chemical Theory and Computation, 2013, 9, 1368-1380.	5.3	69
140	Quantum Mechanical Modeling of Catalytic Processes. Annual Review of Chemical and Biomolecular Engineering, 2011, 2, 453-477.	6.8	68
141	Automated Transition State Searches without Evaluating the Hessian. Journal of Chemical Theory and Computation, 2012, 8, 5166-5174.	5.3	68
142	Selection and Validation of Charge and Lennard-Jones Parameters for QM/MM Simulations of Hydrocarbon Interactions with Zeolites. Journal of Chemical Theory and Computation, 2011, 7, 1695-1703.	5.3	67
143	Computation of high-harmonic generation spectra of H₂and N₂in intense laser pulses using quantum chemistry methods and time-dependent density functional theory. Molecular Physics, 2012, 110, 909-923.	1.7	67
144	Orbital optimized double-hybrid density functionals. Journal of Chemical Physics, 2013, 139, 024110.	3.0	67

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145	Examination of the hydrogen-bonding networks in small water clusters (n = 2â€“5, 13, 17) using absolutely localized molecular orbital energy decomposition analysis. Physical Chemistry Chemical Physics, 2012, 14, 15328.	2.8	66
146	Ab Initio Simulations Reveal that Reaction Dynamics Strongly Affect Product Selectivity for the Cracking of Alkanes over H-MFI. Journal of the American Chemical Society, 2012, 134, 19468-19476.	13.7	66
147	Non-orthogonal configuration interaction for the calculation of multielectron excited states. Journal of Chemical Physics, 2014, 140, 114103.	3.0	66
148	Violations of N-representability from spin-unrestricted orbitals in MÃ¸llerâ€“Plesset perturbation theory and related double-hybrid density functional theory. Molecular Physics, 2009, 107, 1223-1232.	1.7	65
149	Computational Study of p-Xylene Synthesis from Ethylene and 2,5-Dimethylfuran Catalyzed by H-BEA. Journal of Physical Chemistry C, 2014, 118, 22090-22095.	3.1	64
150	The perfect quadruples model for electron correlation in a valence active space. Journal of Chemical Physics, 2009, 130, 084101.	3.0	63
151	Hartree-Fock exchange computed using the atomic resolution of the identity approximation. Journal of Chemical Physics, 2008, 128, 104106.	3.0	62
152	Revisiting the Performance of Time-Dependent Density Functional Theory for Electronic Excitations: Assessment of 43 Popular and Recently Developed Functionals from Rungs One to Four. Journal of Chemical Theory and Computation, 2022, 18, 3460-3473.	5.3	61
153	An efficient method for calculating maxima of homogeneous functions of orthogonal matrices: Applications to localized occupied orbitals. Journal of Chemical Physics, 2004, 121, 9220-9229.	3.0	60
154	Fast evaluation of scaled opposite spin second-order MÃ¸llerâ€“Plesset correlation energies using auxiliary basis expansions and exploiting sparsity. Journal of Computational Chemistry, 2007, 28, 1953-1964.	3.3	59
155	Charge-transfer and the hydrogen bond: Spectroscopic and structural implications from electronic structure calculations. Faraday Discussions, 2011, 150, 345.	3.2	59
156	Insights into the Kinetics of Cracking and Dehydrogenation Reactions of Light Alkanes in H-MFI. Journal of Physical Chemistry C, 2013, 117, 12600-12611.	3.1	59
157	A parallel implementation of the analytic nuclear gradient for time-dependent density functional theory within the Tammâ€“Dancoff approximation. Molecular Physics, 2010, 108, 2791-2800.	1.7	58
158	Approaching closed-shell accuracy for radicals using coupled cluster theory with perturbative triple substitutions. Physical Chemistry Chemical Physics, 2003, 5, 2488.	2.8	57
159	Controlling the Extent of Diradical Character by Utilizing Neighboring Group Interactions. Journal of Physical Chemistry A, 2003, 107, 7475-7481.	2.5	56
160	Variational Energy Decomposition Analysis of Chemical Bonding. 1. Spin-Pure Analysis of Single Bonds. Journal of Chemical Theory and Computation, 2016, 12, 4812-4820.	5.3	56
161	The limits of local correlation theory: Electronic delocalization and chemically smooth potential energy surfaces. Journal of Chemical Physics, 2008, 128, 034103.	3.0	55
162	From Intermolecular Interaction Energies and Observable Shifts to Component Contributions and Back Again: A Tale of Variational Energy Decomposition Analysis. Annual Review of Physical Chemistry, 2021, 72, 641-666.	10.8	55

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163	Configuration interaction with single substitutions for excited states of open-shell molecules. International Journal of Quantum Chemistry, 1995, 56, 361-370.	2.0	54
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