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	Dynamic signatures of electronically nonadiabatic coupling in sodium hydride: a rigorous test for the symmetric quasi-classical model applied to realistic, ab initio electronic states in the adiabatic representation.. Physical Chemistry Chemical Physics, 2022, , .	2.8	5
2	Revisiting the Bonding Model for Gold(I) Species: The Importance of Pauli Repulsion Revealed in a Gold(I)â€Cyclobutadiene Complex. Angewandte Chemie - International Edition, 2022, 61, .	13.8	8
3	Oxygen Isotope Exchange between Carbon Dioxide and Iron Oxides on Marsâ€™ Surface. Journal of Physical Chemistry Letters, 2022, 13, 2600-2606.	4.6	0
4	A Computational and Experimental View of Hydrogen Bonding in Glycerol Water Clusters. Journal of Physical Chemistry A, 2022, 126, 1701-1710.	2.5	3
5	Oxidation State Localized Orbitals: A Method for Assigning Oxidation States Using Optimally Fragment-Localized Orbitals and a Fragment Orbital Localization Index. Journal of Chemical Theory and Computation, 2022, 18, 309-322.	5.3	16
6	Relativistic Orbital-Optimized Density Functional Theory for Accurate Core-Level Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 3438-3449.	4.6	24
7	Pathways for the Formation of C₂₊ Products under Alkaline Conditions during the Electrochemical Reduction of CO₂. ACS Energy Letters, 2022, 7, 1679-1686.	17.4	27
8	Deciphering Distinct Overpotential-Dependent Pathways for Electrochemical CO₂ Reduction Catalyzed by an Ironâ€“Terpyridine Complex. Inorganic Chemistry, 2022, 61, 6919-6933.	4.0	10
9	NewtonNet: a Newtonian message passing network for deep learning of interatomic potentials and forces. , 2022, 1, 333-343.		42
10	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
11	Real-Time Evolution for Ultracompact Hamiltonian Eigenstates on Quantum Hardware. PRX Quantum, 2022, 3, .	9.2	24
12	Computing x-ray absorption spectra from linear-response particles atop optimized holes. Journal of Chemical Physics, 2022, 156, .	3.0	7
13	Concerted Electron-Nuclear Motion in Proton-Coupled Electron Transfer-Driven Grotthuss-Type Proton Translocation. Journal of Physical Chemistry Letters, 2022, , 4479-4485.	4.6	4
14	A benchmark dataset for Hydrogen Combustion. Scientific Data, 2022, 9, 215.	5.3	6
15	Assessing the stability of Pd-exchanged sites in zeolites with the aid of a high throughput quantum chemistry workflow. Nature Communications, 2022, 13, .	12.8	9
16	Copper(III) Metallacyclopentadienes via Zirconocene Transfer and Reductive Elimination to an Isolable Phenanthrocyclobutadiene. Journal of the American Chemical Society, 2022, 144, 9853-9858.	13.7	8
17	Templating Bicarbonate in the Second Coordination Sphere Enhances Electrochemical CO₂ Reduction Catalyzed by Iron Porphyrins. Journal of the American Chemical Society, 2022, 144, 11656-11663.	13.7	45
18	Exchange Coupling Determines Metal-Dependent Efficiency for Iron- and Cobalt-Catalyzed Photochemical CO₂ Reduction. ACS Catalysis, 2022, 12, 8484-8493.	11.2	12

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19	Non-iterative method for constructing valence antibonding molecular orbitals and a molecule-adapted minimum basis. Journal of Chemical Physics, 2022, 157, .	3.0	3
20	Consistent inclusion of continuum solvation in energy decomposition analysis: theory and application to molecular CO₂ reduction catalysts. Chemical Science, 2021, 12, 1398-1414.	7.4	41
21	Modeling Molecules under Pressure with Gaussian Potentials. Journal of Chemical Theory and Computation, 2021, 17, 583-597.	5.3	17
22	A non-perturbative pairwise-additive analysis of charge transfer contributions to intermolecular interaction energies. Physical Chemistry Chemical Physics, 2021, 23, 928-943.	2.8	18
23	Siloxyaluminate and Siloxygallate Complexes as Models for Framework and Partially Hydrolyzed Framework Sites in Zeolites and Zeotypes. Chemistry - A European Journal, 2021, 27, 307-315.	3.3	2
24	Mechanistic Insights into Co and Fe Quaterpyridine-Based CO₂ Reduction Catalysts: Metalâ€“Ligand Orbital Interaction as the Key Driving Force for Distinct Pathways. Journal of the American Chemical Society, 2021, 143, 744-763.	13.7	52
25	Polishing the Gold Standard: The Role of Orbital Choice in CCSD(T) Vibrational Frequency Prediction. Journal of Chemical Theory and Computation, 2021, 17, 742-755.	5.3	18
26	Challenges for density functional theory: calculation of CO adsorption on electrocatalytically relevant metals. Physical Chemistry Chemical Physics, 2021, 23, 9394-9406.	2.8	15
27	Electronâ€“Nuclear Dynamics Accompanying Proton-Coupled Electron Transfer. Journal of the American Chemical Society, 2021, 143, 3104-3112.	13.7	21
28	Mechanism and Kinetics of Light Alkane Dehydrogenation and Cracking over Isolated Ga Species in Ga/H-MFI. ACS Catalysis, 2021, 11, 2062-2075.	11.2	31
29	Too big, too small, or just right? A benchmark assessment of density functional theory for predicting the spatial extent of the electron density of small chemical systems. Journal of Chemical Physics, 2021, 154, 074109.	3.0	15
30	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
31	Controlled Single-Electron Transfer via Metalâ€“Ligand Cooperativity Drives Divergent Nickel-Electrocatalyzed Radical Pathways. Journal of the American Chemical Society, 2021, 143, 6990-7001.	13.7	24
32	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
33	Assessment of Performance of Density Functionals for Predicting Potential Energy Curves in Hydrogen Storage Applications. Journal of Physical Chemistry A, 2021, 125, 4245-4257.	2.5	2
34	Revealing the nature of electron correlation in transition metal complexes with symmetry breaking and chemical intuition. Journal of Chemical Physics, 2021, 154, 194109.	3.0	36
35	Orbital Optimized Density Functional Theory for Electronic Excited States. Journal of Physical Chemistry Letters, 2021, 12, 4517-4529.	4.6	92
36	Two-Coordinate Iron(I) Complexes on the Edge of Stability: Influence of Dispersion and Steric Effects. Organometallics, 2021, 40, 1758-1764.	2.3	6

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37	Critical Role of Thermal Fluctuations for CO Binding on Electrocatalytic Metal Surfaces. Jacs Au, 2021, 1, 1708-1718.	7.9	10
38	Exploring spin symmetry-breaking effects for static field ionization of atoms: Is there an analog to the Coulsonâ€“Fischer point in bond dissociation?. Journal of Chemical Physics, 2021, 155, 014309.	3.0	1
39	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
40	Effective Two-Body Interactions. Journal of Physical Chemistry A, 2021, 125, 7750-7758.	2.5	11
41	Exploring the Limits of Second- and Third-Order MÃ¸llerâ€“Plesset Perturbation Theories for Noncovalent Interactions: Revisiting MP2.5 and Assessing the Importance of Regularization and Reference Orbitals. Journal of Chemical Theory and Computation, 2021, 17, 5582-5599.	5.3	11
42	The Role of Roughening to Enhance Selectivity to C₂₊ Products during CO₂ Electroreduction on Copper. ACS Energy Letters, 2021, 6, 3252-3260.	17.4	38
43	Observation of an Intermediate to H₂ Binding in a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2021, 143, 14884-14894.	13.7	32
44	Computational modeling predicts the stability of both Pd⁺ and Pd²⁺ ion-exchanged into H-CHA. Journal of Materials Chemistry A, 2021, 9, 2161-2174.	10.3	20
45	Optimized Pseudopotentials and Basis Sets for Semiempirical Density Functional Theory for Electrocatalysis Applications. Journal of Physical Chemistry Letters, 2021, 12, 10304-10309.	4.6	12
46	Molecular magnetisabilities computed via finite fields: assessing alternatives to MP2 and revisiting magnetic exaltations in aromatic and antiaromatic species. Molecular Physics, 2021, 119, .	1.7	1
47	Approaching the basis set limit in Gaussian-orbital-based periodic calculations with transferability: Performance of pure density functionals for simple semiconductors. Journal of Chemical Physics, 2021, 155, 164102.	3.0	14
48	Crossed Beam Experiments and Computational Studies of Pathways to the Preparation of Singlet Ethynylsilylene (HCCSiH; X1Aâ€²): The Silacarbene Counterpart of Triplet Propargylene (HCCCH; X3B). Journal of Physical Chemistry Letters, 2021, 12, 10768-10776.	4.6	4
49	Stripping away ion hydration shells in electrical double-layer formation: Water networks matter. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	20
50	Dissociation of HCl in water nanoclusters: an energy decomposition analysis perspective. Physical Chemistry Chemical Physics, 2021, 23, 26737-26749.	2.8	1
51	Regularized Second-Order MÃ¸llerâ€“Plesset Theory: A More Accurate Alternative to Conventional MP2 for Noncovalent Interactions and Transition Metal Thermochemistry for the Same Computational Cost. Journal of Physical Chemistry Letters, 2021, 12, 12084-12097.	4.6	32
52	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
53	Variational Forwardâ€“Backward Charge Transfer Analysis Based on Absolutely Localized Molecular Orbitals: Energetics and Molecular Properties. Journal of Chemical Theory and Computation, 2020, 16, 1073-1089.	5.3	21
54	Electronic structure calculations permit identification of the driving forces behind frequency shifts in transition metal monocarbonyls. Physical Chemistry Chemical Physics, 2020, 22, 781-798.	2.8	21

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55	Systematically Improvable Tensor Hypercontraction: Interpolative Separable Density-Fitting for Molecules Applied to Exact Exchange, Second- and Third-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2020, 16, 243-263.	5.3	44
56	Facing the Challenges of Borderline Oxidation State Assignments Using State-of-the-Art Computational Methods. Inorganic Chemistry, 2020, 59, 15410-15420.	4.0	27
57	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
58	Accurate prediction of core-level spectra of radicals at density functional theory cost via square gradient minimization and recoupling of mixed configurations. Journal of Chemical Physics, 2020, 153, 134108.	3.0	31
59	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
60	Predicting Excitation Energies of Twisted Intramolecular Charge-Transfer States with the Time-Dependent Density Functional Theory: Comparison with Experimental Measurements in the Gas Phase and Solvents Ranging from Hexanes to Acetonitrile. Journal of Chemical Theory and Computation, 2020, 16, 6244-6255.	5.3	21
61	Molecular growth upon ionization of van der Waals clusters containing HCCH and HCN is a pathway to prebiotic molecules. Physical Chemistry Chemical Physics, 2020, 22, 20337-20348.	2.8	8
62	Third-Order MÃ¸llerâ€“Plesset Theory Made More Useful? The Role of Density Functional Theory Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 7473-7489.	5.3	27
63	Solvent Mediated Excited State Proton Transfer in Indigo Carmine. Journal of Physical Chemistry Letters, 2020, 11, 4156-4162.	4.6	26
64	Probing radicalâ€“molecule interactions with a second generation energy decomposition analysis of DFT calculations using absolutely localized molecular orbitals. Physical Chemistry Chemical Physics, 2020, 22, 12867-12885.	2.8	17
65	Computational Study of an Iron(II) Polypyridine Electrocatalyst for CO₂ Reduction: Key Roles for Intramolecular Interactions in CO₂ Binding and Proton Transfer. Inorganic Chemistry, 2020, 59, 8146-8160.	4.0	23
66	Bimetallic Mechanism for Alkyne Cyclotrimerization with a Two-Coordinate Fe Precatalyst. ACS Catalysis, 2020, 10, 7800-7807.	11.2	14
67	The rupture mechanism of rubredoxin is more complex than previously thought. Chemical Science, 2020, 11, 6036-6044.	7.4	1
68	Benchmarking the Performance of the ReaxFF Reactive Force Field on Hydrogen Combustion Systems. Journal of Physical Chemistry A, 2020, 124, 5631-5645.	2.5	28
69	Compressed intramolecular dispersion interactions. Journal of Chemical Physics, 2020, 152, 024112.	3.0	2
70	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
71	Experimental and Computational Studies of Carbonâ€“Carbon Bond Formation via Ketonization and Aldol Condensation over Site-Isolated Zirconium Catalysts. ACS Catalysis, 2020, 10, 4566-4579.	11.2	33
72	Density Functionals for Hydrogen Storage: Defining the H2Bind275 Test Set with Ab Initio Benchmarks and Assessment of 55 Functionals. Journal of Chemical Theory and Computation, 2020, 16, 4963-4982.	5.3	14

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73	Cation, Anion, and Radical Isomers of C4H4N: Computational Characterization and Implications for Astrophysical and Planetary Environments. Journal of Physical Chemistry A, 2020, 124, 2001-2013.	2.5	12
74	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
75	Heterogenized Pyridine-Substituted Cobalt(II) Phthalocyanine Yields Reduction of CO₂ by Tuning the Electron Affinity of the Co Center. ACS Applied Materials & Interfaces, 2020, 12, 5251-5258.	8.0	41
76	Atomicâ€Scale Spacing between Copper Facets for the Electrochemical Reduction of Carbon Dioxide. Advanced Energy Materials, 2020, 10, 1903423.	19.5	32
77	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
78	Generalized single excitation configuration interaction: an investigation into the impact of the inclusion of non-orthogonality on the calculation of core-excited states. Physical Chemistry Chemical Physics, 2020, 22, 8182-8192.	2.8	16
79	Clarifying the quantum mechanical origin of the covalent chemical bond. Nature Communications, 2020, 11, 4893.	12.8	34
80	Development of an Advanced Force Field for Water Using Variational Energy Decomposition Analysis. Journal of Chemical Theory and Computation, 2019, 15, 5001-5013.	5.3	49
81	Two single-reference approaches to singlet biradicaloid problems: Complex, restricted orbitals and approximate spin-projection combined with regularized orbital-optimized MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2019, 150, 244106.	3.0	36
82	Multiresolution 3D-DenseNet for Chemical Shift Prediction in NMR Crystallography. Journal of Physical Chemistry Letters, 2019, 10, 4558-4565.	4.6	38
83	Chemoenzymatic Platform for Synthesis of Chiral Organofluorines Based on Typeâ€…II Aldolases. Angewandte Chemie, 2019, 131, 11967-11971.	2.0	14
84	Gas phase formation of c-SiC ₃ molecules in the circumstellar envelope of carbon stars. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14471-14478.	7.1	19
85	Third-Order MÃ¸llerâ€“Plesset Perturbation Theory Made Useful? Choice of Orbitals and Scaling Greatly Improves Accuracy for Thermochemistry, Kinetics, and Intermolecular Interactions. Journal of Physical Chemistry Letters, 2019, 10, 4170-4176.	4.6	33
86	Energy Decomposition Analysis for Interactions of Radicals: Theory and Implementation at the MP2 Level with Application to Hydration of Halogenated Benzene Cations and Complexes between CO₂^{â€“}Â· and Pyridine and Imidazole. Journal of Physical Chemistry A, 2019, 123, 9621-9633.	2.5	12
87	Quantum Chemical Modeling of Pressureâ€Induced Spin Crossover in Octahedral Metalâ€Ligand Complexes. ChemPhysChem, 2019, 20, 2742-2747.	2.1	14
88	What Levels of Coupled Cluster Theory Are Appropriate for Transition Metal Systems? A Study Using Near-Exact Quantum Chemical Values for 3d Transition Metal Binary Compounds. Journal of Chemical Theory and Computation, 2019, 15, 5370-5385.	5.3	42
89	Kohn-Sham Density Functional Theory with Complex, Spin-Restricted Orbitals: Accessing a New Class of Densities without the Symmetry Dilemma. Physical Review Letters, 2019, 123, 113001.	7.8	21
90	Probing solvation and reactivity in ionized polycyclic aromatic hydrocarbonâ€“water clusters with photoionization mass spectrometry and electronic structure calculations. Faraday Discussions, 2019, 217, 414-433.	3.2	18

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91	Chemoenzymatic Platform for Synthesis of Chiral Organofluorines Based on Typeâ€…II Aldolases. Angewandte Chemie - International Edition, 2019, 58, 11841-11845.	13.8	34
92	Assessing Electronic Structure Methods for Long-Range Three-Body Dispersion Interactions: Analysis and Calculations on Well-Separated Metal Atom Trimers. Journal of Chemical Theory and Computation, 2019, 15, 4351-4361.	5.3	7
93	Probing Blue-Shifting Hydrogen Bonds with Adiabatic Energy Decomposition Analysis. Journal of Physical Chemistry Letters, 2019, 10, 3899-3905.	4.6	27
94	Zeolite-Catalyzed Isobutene Amination: Mechanism and Kinetics. ACS Catalysis, 2019, 9, 7012-7022.	11.2	19
95	Non-Orthogonal Configuration Interaction with Single Substitutions for Core-Excited States: An Extension to Doublet Radicals. Journal of Chemical Theory and Computation, 2019, 15, 2966-2973.	5.3	39
96	Tracing the 267 nm-Induced Radical Formation in Dimethyl Disulfide Using Time-Resolved X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 1382-1387.	4.6	24
97	Mutually polarizable QM/MM model with in situ optimized localized basis functions. Journal of Chemical Physics, 2019, 150, 074103.	3.0	16
98	Well-behaved versus ill-behaved density functionals for single bond dissociation: Separating success from disaster functional by functional for stretched H2. Journal of Chemical Physics, 2019, 150, 094115.	3.0	25
99	Distinguishing artificial and essential symmetry breaking in a single determinant: approach and application to the C₆₀, C₃₆, and C₂₀ fullerenes. Physical Chemistry Chemical Physics, 2019, 21, 4763-4778.	2.8	40
100	Explaining the Incorporation of Oxygen Derived from Solvent Water into the Oxygenated Products of CO Reduction over Cu. Journal of the American Chemical Society, 2019, 141, 4191-4193.	13.7	29
101	The Poissonâ€“Boltzmann model for implicit solvation of electrolyte solutions: Quantum chemical implementation and assessment via Sechenov coefficients. Journal of Chemical Physics, 2019, 151, 224111.	3.0	24
102	Beyond the Coulsonâ€“Fischer point: characterizing single excitation CI and TDDFT for excited states in single bond dissociations. Physical Chemistry Chemical Physics, 2019, 21, 21761-21775.	2.8	20
103	Making many-body interactions nearly pairwise additive: The polarized many-body expansion approach. Journal of Chemical Physics, 2019, 151, 194101.	3.0	18
104	Excited states via coupled cluster theory without equation-of-motion methods: Seeking higher roots with application to doubly excited states and double core hole states. Journal of Chemical Physics, 2019, 151, 214103.	3.0	45
105	Mechanism and Kinetics of Propane Dehydrogenation and Cracking over Ga/H-MFI Prepared via Vapor-Phase Exchange of H-MFI with GaCl₃. Journal of the American Chemical Society, 2019, 141, 1614-1627.	13.7	107
106	Push it to the limit: comparing periodic and local approaches to density functional theory for intermolecular interactions. Molecular Physics, 2019, 117, 1298-1305.	1.7	6
107	Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. ACS Catalysis, 2019, 9, 920-931.	11.2	153
108	Generalized Unitary Coupled Cluster Wave functions for Quantum Computation. Journal of Chemical Theory and Computation, 2019, 15, 311-324.	5.3	260

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109	Understanding BrÃ¸nsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. ChemPhysChem, 2018, 19, 338-338.	2.1	0
110	On the Computational Characterization of Charge-Transfer Effects in Noncovalently Bound Molecular Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2401-2417.	5.3	51
111	Energy decomposition analysis for exciplexes using absolutely localized molecular orbitals. Journal of Chemical Physics, 2018, 148, 064105.	3.0	36
112	Impact of long-range electrostatic and dispersive interactions on theoretical predictions of adsorption and catalysis in zeolites. Catalysis Today, 2018, 312, 51-65.	4.4	35
113	Is Subsurface Oxygen Necessary for the Electrochemical Reduction of CO₂ on Copper?. Journal of Physical Chemistry Letters, 2018, 9, 601-606.	4.6	118
114	Mechanism of CO₂ Reduction at Copper Surfaces: Pathways to C₂ Products. ACS Catalysis, 2018, 8, 1490-1499.	11.2	608
115	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
116	Understanding BrÃ¸nstedâ€Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. ChemPhysChem, 2018, 19, 341-358.	2.1	21
117	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
118	Orbital optimisation in the perfect pairing hierarchy: applications to full-valence calculations on linear polyacenes. Molecular Physics, 2018, 116, 547-560.	1.7	17
119	Independent amplitude approximations in coupled cluster valence bond theory: Incorporation of 3-electron-pair correlation and application to spin frustration in the low-lying excited states of a ferredoxin-type tetrametallic iron-sulfur cluster. Journal of Chemical Physics, 2018, 149, 144103.	3.0	7
120	Open-shell coupled-cluster valence-bond theory augmented with an independent amplitude approximation for three-pair correlations: Application to a model oxygen-evolving complex and single molecular magnet. Journal of Chemical Physics, 2018, 149, 244121.	3.0	13
121	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
122	Energy Decomposition Analysis for Excimers Using Absolutely Localized Molecular Orbitals within Time-Dependent Density Functional Theory and Configuration Interaction with Single Excitations. Journal of Chemical Theory and Computation, 2018, 14, 5156-5168.	5.3	22
123	Resonance-stabilized hydrocarbon-radical chain reactions may explain soot inception and growth. Science, 2018, 361, 997-1000.	12.6	472
124	Reaction mechanism of the selective reduction of CO₂ to CO by a tetraaza [Co^{II}N₄H]²⁺ complex in the presence of protons. Physical Chemistry Chemical Physics, 2018, 20, 24058-24064.	2.8	15
125	Unraveling substituent effects on frontier orbitals of conjugated molecules using an absolutely localized molecular orbital based analysis. Chemical Science, 2018, 9, 8598-8607.	7.4	46
126	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

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127	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
128	Non-orthogonal configuration interaction with single substitutions for the calculation of core-excited states. Journal of Chemical Physics, 2018, 149, 044116.	3.0	44
129	Efficient Implementation of NOCI-MP2 Using the Resolution of the Identity Approximation with Application to Charged Dimers and Long Câ€“C Bonds in Ethane Derivatives. Journal of Chemical Theory and Computation, 2018, 14, 4791-4805.	5.3	18
130	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
131	Understanding Non-Covalent Interactions: Correlated Energy Decomposition Analysis and Applications to Halogen Bonding. Chimia, 2018, 72, 193.	0.6	7
132	Nonempirical Meta-Generalized Gradient Approximations for Modeling Chemisorption at Metal Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 3083-3090.	5.3	20
133	Communication: xDH double hybrid functionals can be qualitatively incorrect for non-equilibrium geometries: Dipole moment inversion and barriers to radical-radical association using XYG3 and XYGJ-OS. Journal of Chemical Physics, 2018, 148, 171102.	3.0	20
134	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
135	Bimolecular Reaction Dynamics in the Phenylâ€“Silane System: Exploring the Prototype of a Radical Substitution Mechanism. Journal of Physical Chemistry Letters, 2018, 9, 5135-5142.	4.6	3
136	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
137	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
138	Coupled-Cluster Valence-Bond Singles and Doubles for Strongly Correlated Systems: Block-Tensor Based Implementation and Application to Oligoacenes. Journal of Chemical Theory and Computation, 2017, 13, 602-615.	5.3	54
139	A General Sparse Tensor Framework for Electronic Structure Theory. Journal of Chemical Theory and Computation, 2017, 13, 1108-1116.	5.3	10
140	Ab initio molecular dynamics simulations of liquid water using high quality meta-GGA functionals. Chemical Science, 2017, 8, 3554-3565.	7.4	95
141	Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation ofn-Butane in BrÃ¸nsted Acidic Zeolites. ACS Catalysis, 2017, 7, 2685-2697.	11.2	42
142	Energy decomposition analysis in an adiabatic picture. Physical Chemistry Chemical Physics, 2017, 19, 5944-5958.	2.8	54
143	Simulating the absorption spectra of helium clusters (Nâ€‰=â€‰70, 150, 231, 300) using a charge transfer correction to superposition of fragment single excitations. Journal of Chemical Physics, 2017, 146, 044111.	3.0	11
144	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

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145	Stabilizing potentials in bound state analytic continuation methods for electronic resonances in polyatomic molecules. Journal of Chemical Physics, 2017, 146, 044112.	3.0	16
146	Performance of the AMOEBA Water Model in the Vicinity of QM Solutes: A Diagnosis Using Energy Decomposition Analysis. Journal of Chemical Theory and Computation, 2017, 13, 1963-1979.	5.3	28
147	Quantifying the Role of Orbital Contraction in Chemical Bonding. Journal of Physical Chemistry Letters, 2017, 8, 1967-1972.	4.6	20
148	Ab initio dynamics and photoionization mass spectrometry reveal ionâ€“molecule pathways from ionized acetylene clusters to benzene cation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E4125-E4133.	7.1	24
149	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
150	Methane Storage: Molecular Mechanisms Underlying Room-Temperature Adsorption in Zn₄O(BDC)₃ (MOF-5). Journal of Physical Chemistry C, 2017, 121, 12091-12100.	3.1	28
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