John M Herbert

List of Publications by Year
in descending order

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136 papers	12,773 citations	34100 52 h-index	24254 110 g-index
168 all docs	168 docs citations	168 times ranked	9471 citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
3	A long-range-corrected density functional that performs well for both ground-state properties and time-dependent density functional theory excitation energies, including charge-transfer excited states. Journal of Chemical Physics, 2009, 130, 054112.	3.0	566
4	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
5	Simultaneous benchmarking of ground- and excited-state properties with long-range-corrected density functional theory. Journal of Chemical Physics, 2008, 129, 034107.	3.0	287
6	A generalized many-body expansion and a unified view of fragment-based methods in electronic structure theory. Journal of Chemical Physics, 2012, 137, 064113.	3.0	184
7	Both Intra- and Interstrand Charge-Transfer Excited States in Aqueous B-DNA Are Present at Energies Comparable To, or Just Above, the ¹Ï€Ï€* Excitonic Bright States. Journal of the American Chemical Society, 2009, 131, 3913-3922.	13.7	177
8	Charge-Transfer Excited States in a Ï€-Stacked Adenine Dimer, As Predicted Using Long-Range-Corrected Time-Dependent Density Functional Theory. Journal of Physical Chemistry B, 2008, 112, 6304-6308.	2.6	165
9	A smooth, nonsingular, and faithful discretization scheme for polarizable continuum models: The switching/Gaussian approach. Journal of Chemical Physics, 2010, 133, 244111.	3.0	165
10	Time-Dependent Density-Functional Description of the ¹L_a State in Polycyclic Aromatic Hydrocarbons: Charge-Transfer Character in Disguise?. Journal of Chemical Theory and Computation, 2011, 7, 1296-1306.	5.3	164
11	Calculation of Electron Detachment Energies for Water Cluster Anions:Â An Appraisal of Electronic Structure Methods, with Application to (H2O)20-and (H2O)24-. Journal of Physical Chemistry A, 2005, 109, 5217-5229.	2.5	139
12	The Hydrated Electron. Annual Review of Physical Chemistry, 2017, 68, 447-472.	10.8	136
13	Experimental Benchmark Data and Systematic Evaluation of Two a Posteriori, Polarizable-Continuum Corrections for Vertical Excitation Energies in Solution. Journal of Physical Chemistry A, 2015, 119, 5446-5464.	2.5	120
14	Polarizable Continuum Reaction-Field Solvation Models Affording Smooth Potential Energy Surfaces. Journal of Physical Chemistry Letters, 2010, 1, 556-561.	4.6	103
15	Fantasy versus reality in fragment-based quantum chemistry. Journal of Chemical Physics, 2019, 151, 170901.	3.0	102
16	Noncovalent Interactions in Extended Systems Described by the Effective Fragment Potential Method: Theory and Application to Nucleobase Oligomers. Journal of Physical Chemistry A, 2010, 114, 12739-12754.	2.5	100
17	Accelerated, energy-conserving Bornâ€“Oppenheimer molecular dynamics via Fock matrix extrapolation. Physical Chemistry Chemical Physics, 2005, 7, 3269.	2.8	96
18	Simple Methods To Reduce Charge-Transfer Contamination in Time-Dependent Density-Functional Calculations of Clusters and Liquids. Journal of Chemical Theory and Computation, 2007, 3, 1680-1690.	5.3	93

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19	Aiming for Benchmark Accuracy with the Many-Body Expansion. Accounts of Chemical Research, 2014, 47, 2828-2836.	15.6	92
20	Evidence for Singlet Fission Driven by Vibronic Coherence in Crystalline Tetracene. Journal of Physical Chemistry Letters, 2017, 8, 1442-1448.	4.6	91
21	Dielectric continuum methods for quantum chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1519.	14.6	91
22	Accurate Description of Intermolecular Interactions Involving Ions Using Symmetry-Adapted Perturbation Theory. Journal of Chemical Theory and Computation, 2015, 11, 2473-2486.	5.3	90
23	A one-electron model for the aqueous electron that includes many-body electron-water polarization: Bulk equilibrium structure, vertical electron binding energy, and optical absorption spectrum. Journal of Chemical Physics, 2010, 133, 154506.	3.0	89
24	Analytic derivative couplings for spin-flip configuration interaction singles and spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2014, 141, 064104.	3.0	89
25	Accuracy and limitations of second-order many-body perturbation theory for predicting vertical detachment energies of solvated-electron clusters. Physical Chemistry Chemical Physics, 2006, 8, 68-78.	2.8	84
26	An efficient, fragment-based electronic structure method for molecular systems: Self-consistent polarization with perturbative two-body exchange and dispersion. Journal of Chemical Physics, 2011, 134, 094118.	3.0	82
27	Accurate and Efficient Quantum Chemistry Calculations for Noncovalent Interactions in Many-Body Systems: The XSAPT Family of Methods. Journal of Physical Chemistry A, 2015, 119, 235-252.	2.5	82
28	Comment on â€œDoes the Hydrated Electron Occupy a Cavity?â€• Science, 2011, 331, 1387-1387.	12.6	78
29	Understanding the many-body expansion for large systems. I. Precision considerations. Journal of Chemical Physics, 2014, 141, 014108.	3.0	77
30	Energy Decomposition Analysis with a Stable Charge-Transfer Term for Interpreting Intermolecular Interactions. Journal of Chemical Theory and Computation, 2016, 12, 2569-2582.	5.3	75
31	Beyond Time-Dependent Density Functional Theory Using Only Single Excitations: Methods for Computational Studies of Excited States in Complex Systems. Accounts of Chemical Research, 2016, 49, 931-941.	15.6	75
32	Ab Initio Implementation of the Frenkelâ€“Davydov Exciton Model: A Naturally Parallelizable Approach to Computing Collective Excitations in Crystals and Aggregates. Journal of Chemical Theory and Computation, 2014, 10, 5366-5376.	5.3	74
33	Standard grids for highâ€precision integration of modern density functionals: SGâ€2 and SGâ€3. Journal of Computational Chemistry, 2017, 38, 869-882.	3.3	70
34	Structure of the Aqueous Electron: Assessment of One-Electron Pseudopotential Models in Comparison to Experimental Data and Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2011, 115, 14470-14483.	2.5	69
35	Symmetric versus asymmetric discretization of the integral equations in polarizable continuum solvation models. Chemical Physics Letters, 2011, 509, 77-87.	2.6	67
36	Curvy-steps approach to constraint-free extended-Lagrangian ab initio molecular dynamics, using atom-centered basis functions: Convergence toward Bornâ€“Oppenheimer trajectories. Journal of Chemical Physics, 2004, 121, 11542-11556.	3.0	65

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37	Understanding the many-body expansion for large systems. II. Accuracy considerations. Journal of Chemical Physics, 2016, 144, 164105.	3.0	65
38	Time-resolved infrared spectroscopy of the lowest triplet state of thymine and thymidine. Chemical Physics, 2008, 347, 383-392.	1.9	64
39	On the accuracy of the general, state-specific polarizable-continuum model for the description of correlated ground- and excited states in solution. Physical Chemistry Chemical Physics, 2017, 19, 1644-1654.	2.8	62
40	State-Targeted Energy Projection: A Simple and Robust Approach to Orbital Relaxation of Non-Aufbau Self-Consistent Field Solutions. Journal of Chemical Theory and Computation, 2020, 16, 5067-5082.	5.3	62
41	Reinterpreting Ï€-stacking. Physical Chemistry Chemical Physics, 2020, 22, 24870-24886.	2.8	62
42	Optical Spectroscopy of the Bulk and Interfacial Hydrated Electron from Ab Initio Calculations. Journal of Physical Chemistry A, 2014, 118, 7507-7515.	2.5	61
43	An improved treatment of empirical dispersion and a many-body energy decomposition scheme for the explicit polarization plus symmetry-adapted perturbation theory (XSAPT) method. Journal of Chemical Physics, 2013, 139, 034107.	3.0	60
44	Analytic derivative couplings in time-dependent density functional theory: Quadratic response theory versus pseudo-wavefunction approach. Journal of Chemical Physics, 2015, 142, 064109.	3.0	60
45	Charge Penetration and the Origin of Large Oâˆ'H Vibrational Red-Shifts in Hydrated-Electron Clusters, (H2O)n-. Journal of the American Chemical Society, 2006, 128, 13932-13939.	13.7	59
46	Theoretical Characterization of Four Distinct Isomer Types in Hydrated-Electron Clusters, and Proposed Assignments for Photoelectron Spectra of Water Cluster Anions. Journal of the American Chemical Society, 2011, 133, 19889-19899.	13.7	57
47	Many-Body Expansion with Overlapping Fragments: Analysis of Two Approaches. Journal of Chemical Theory and Computation, 2013, 9, 1408-1416.	5.3	57
48	Spin-flip, tensor equation-of-motion configuration interaction with a density-functional correction: A spin-complete method for exploring excited-state potential energy surfaces. Journal of Chemical Physics, 2015, 143, 234107.	3.0	57
49	Electrostatics does not dictate the slip-stacked arrangement of aromatic Ï€â€“Ï€ interactions. Chemical Science, 2020, 11, 6758-6765.	7.4	57
50	Rapid computation of intermolecular interactions in molecular and ionic clusters: self-consistent polarization plus symmetry-adapted perturbation theory. Physical Chemistry Chemical Physics, 2012, 14, 7679.	2.8	56
51	The Hydrated Electron at the Surface of Neat Liquid Water Appears To Be Indistinguishable from the Bulk Species. Journal of the American Chemical Society, 2016, 138, 10879-10886.	13.7	56
52	First-principles, quantum-mechanical simulations of electron solvation by a water cluster. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 14282-14287.	7.1	55
53	Polarization-Bound Quasi-Continuum States Are Responsible for the â€œBlue Tailâ€• in the Optical Absorption Spectrum of the Aqueous Electron. Journal of the American Chemical Society, 2010, 132, 10000-10002.	13.7	55
54	Accurate Intermolecular Interactions at Dramatically Reduced Cost: XPol+SAPT with Empirical Dispersion. Journal of Physical Chemistry Letters, 2012, 3, 3241-3248.	4.6	54

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55	Structure of the aqueous electron. Physical Chemistry Chemical Physics, 2019, 21, 20538-20565.	2.8	54
56	N-representability and variational stability in natural orbital functional theory. Journal of Chemical Physics, 2003, 118, 10835-10846.	3.0	53
57	Comparison of the Marcus and Pekar partitions in the context of non-equilibrium, polarizable-continuum solvation models. Journal of Chemical Physics, 2015, 143, 204104.	3.0	52
58	Pairâ€“Pair Approximation to the Generalized Many-Body Expansion: An Alternative to the Four-Body Expansion for ab Initio Prediction of Protein Energetics via Molecular Fragmentation. Journal of Chemical Theory and Computation, 2016, 12, 572-584.	5.3	52
59	Accurate and Efficient ab Initio Calculations for Supramolecular Complexes: Symmetry-Adapted Perturbation Theory with Many-Body Dispersion. Journal of Physical Chemistry Letters, 2019, 10, 2706-2714.	4.6	51
60	Nature's most squishy ion: The important role of solvent polarization in the description of the hydrated electron. International Reviews in Physical Chemistry, 2011, 30, 1-48.	2.3	48
61	Energy-Screened Many-Body Expansion: A Practical Yet Accurate Fragmentation Method for Quantum Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 475-487.	5.3	48
62	The static-exchange electron-water pseudopotential, in conjunction with a polarizable water model: A new Hamiltonian for hydrated-electron simulations. Journal of Chemical Physics, 2009, 130, 124115.	3.0	47
63	Excited-State Deactivation Pathways in Uracil versus Hydrated Uracil: Solvatochromatic Shift in the ¹nÏ€* State is the Key. Journal of Physical Chemistry B, 2014, 118, 7806-7817.	2.6	47
64	Atomic Orbital Implementation of Extended Symmetry-Adapted Perturbation Theory (XSAPT) and Benchmark Calculations for Large Supramolecular Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2955-2978.	5.3	43
65	Periodic boundary conditions for QM/MM calculations: Ewald summation for extended Gaussian basis sets. Journal of Chemical Physics, 2013, 139, 244108.	3.0	42
66	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. Journal of Chemical Theory and Computation, 2016, 12, 332-344.	5.3	42
67	Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study. Journal of Molecular Liquids, 2020, 297, 111902.	4.9	42
68	Adiabatic diffusion Monte Carlo approaches for studies of ground and excited state properties of van der Waals complexes. Journal of Chemical Physics, 1999, 110, 5481-5484.	3.0	40
69	Stabilization and rovibronic spectra of the T-shaped and linear ground-state conformers of a weakly bound rare-gasâ€“homonuclear dihalogen complex: Heâ‹¯Br2. Journal of Chemical Physics, 2005, 123, 104312.	3.0	40
70	Achieving the CCSD(T) Basis-Set Limit in Sizable Molecular Clusters: Counterpoise Corrections for the Many-Body Expansion. Journal of Physical Chemistry Letters, 2013, 4, 2674-2680.	4.6	40
71	Ab Initio Investigation of Electron Detachment in Dicarboxylate Dianions. Journal of Physical Chemistry A, 2000, 104, 11786-11795.	2.5	39
72	Breakdown of the Single-Exchange Approximation in Third-Order Symmetry-Adapted Perturbation Theory. Journal of Physical Chemistry A, 2012, 116, 3042-3047.	2.5	38

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73	Efficient Monomer-Based Quantum Chemistry Methods for Molecular and Ionic Clusters. Annual Reports in Computational Chemistry, 2013, 9, 25-58.	1.7	37
74	Low-Scaling Quantum Chemistry Approach to Excited-State Properties via an ab Initio Exciton Model: Application to Excitation Energy Transfer in a Self-Assembled Nanotube. Journal of Physical Chemistry Letters, 2015, 6, 4390-4396.	4.6	37
75	Infrared photodissociation of a water molecule from a flexible molecule-H2O complex: Rates and conformational product yields following XH stretch excitation. Journal of Chemical Physics, 2007, 126, 134306.	3.0	35
76	Self-consistent predictor/corrector algorithms for stable and efficient integration of the time-dependent Kohn-Sham equation. Journal of Chemical Physics, 2018, 148, 044117.	3.0	35
77	Influence of Structure on Electron Correlation Effects and Electronâ"Water Dispersion Interactions in Anionic Water Clusters. Journal of Physical Chemistry A, 2008, 112, 6171-6178.	2.5	34
78	Analytic gradient for the QM/MM-Ewald method using charges derived from the electrostatic potential: Theory, implementation, and application to ab initio molecular dynamics simulation of the aqueous electron. Journal of Chemical Physics, 2019, 150, 144115.	3.0	34
79	Symmetry-adapted perturbation theory with Kohn-Sham orbitals using non-empirically tuned, long-range-corrected density functionals. Journal of Chemical Physics, 2014, 140, 044108.	3.0	30
80	Understanding the many-body expansion for large systems. III. Critical role of four-body terms, counterpoise corrections, and cutoffs. Journal of Chemical Physics, 2017, 147, 161729.	3.0	30
81	Quantum chemistry in arbitrary dielectric environments: Theory and implementation of nonequilibrium Poisson boundary conditions and application to compute vertical ionization energies at the air/water interface. Journal of Chemical Physics, 2018, 148, 222834.	3.0	29
82	Approaching the complete-basis limit with a truncated many-body expansion. Journal of Chemical Physics, 2013, 139, 224102.	3.0	28
83	An efficient and accurate approximation to time-dependent density functional theory for systems of weakly coupled monomers. Journal of Chemical Physics, 2015, 143, 034106.	3.0	27
84	Extensivity and the contracted SchrÃ¶dinger equation. Journal of Chemical Physics, 2002, 117, 7464-7471.	3.0	26
85	Contraction relations for Grassmann products of reduced density matrices and implications for density matrix reconstruction. Physical Review A, 2002, 65, .	2.5	25
86	Ab Initio Investigation of the Resonance Raman Spectrum of the Hydrated Electron. Journal of Physical Chemistry B, 2019, 123, 8074-8085.	2.6	25
87	Charge Separation and Charge Transfer in the Low-Lying Excited States of Pentacene. Journal of Physical Chemistry C, 2020, 124, 24653-24666.	3.1	25
88	Unimolecular Rearrangement oftrans-FONO to FNO2. A Possible Model System for Atmospheric Nitrate Formationâ€. Journal of Physical Chemistry A, 2004, 108, 7639-7642.	2.5	24
89	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
90	Comparison of two-electron densities reconstructed from one-electron density matrices. International Journal of Quantum Chemistry, 2002, 90, 355-369.	2.0	23

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91	Interaction of Graphene Quantum Dots with Oligothiophene: A Comprehensive Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 29556-29570.	3.1	22
92	Predicting and Understanding Non-Covalent Interactions Using Novel Forms of Symmetry-Adapted Perturbation Theory. Accounts of Chemical Research, 2021, 54, 3679-3690.	15.6	22
93	Improving Generalized Born Models by Exploiting Connections to Polarizable Continuum Models. I. An Improved Effective Coulomb Operator. Journal of Chemical Theory and Computation, 2012, 8, 1999-2011.	5.3	21
94	A Structural Model for a Self-Assembled Nanotube Provides Insight into Its Exciton Dynamics. Journal of Physical Chemistry C, 2015, 119, 13948-13956.	3.1	21
95	Analytic derivative couplings and first-principles exciton/phonon coupling constants for an ab initio Frenkel-Davydov exciton model: Theory, implementation, and application to compute triplet exciton mobility parameters for crystalline tetracene. Journal of Chemical Physics, 2017, 146, 224110.	3.0	21
96	Neat, Simple, and Wrong: Debunking Electrostatic Fallacies Regarding Noncovalent Interactions. Journal of Physical Chemistry A, 2021, 125, 7125-7137.	2.5	21
97	Magnitude and significance of the higher-order reduced density matrix cumulants. International Journal of Quantum Chemistry, 2007, 107, 703-711.	2.0	20
98	What Is the Price of Open-Source Software?. Journal of Physical Chemistry Letters, 2015, 6, 2751-2754.	4.6	19
99	Local Excitation Approximations to Time-Dependent Density Functional Theory for Excitation Energies in Solution. Journal of Chemical Theory and Computation, 2016, 12, 157-166.	5.3	19
100	A Simple Correction for Nonadditive Dispersion within Extended Symmetry-Adapted Perturbation Theory (XSAPT). Journal of Chemical Theory and Computation, 2018, 14, 5128-5142.	5.3	19
101	Variational Formulation of the Generalized Many-Body Expansion with Self-Consistent Charge Embedding: Simple and Correct Analytic Energy Gradient for Fragment-Basedab InitioMolecular Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 3877-3886.	4.6	19
102	A simple polarizable continuum solvation model for electrolyte solutions. Journal of Chemical Physics, 2011, 134, 204110.	3.0	18
103	Reparameterization of an Accurate, Few-Parameter Implicit Solvation Model for Quantum Chemistry: Composite Method for Implicit Representation of Solvent, CMIRS v. 1.1. Journal of Chemical Theory and Computation, 2016, 12, 4338-4346.	5.3	18
104	Self-interaction in natural orbital functional theory. Chemical Physics Letters, 2003, 382, 142-149.	2.6	17
105	What Is the Optoelectronic Effect of the Capsule on the Guest Molecule in Aqueous Host/Guest Complexes? A Combined Computational and Spectroscopic Perspective. Journal of Physical Chemistry C, 2017, 121, 15481-15488.	3.1	17
106	Self-consistent charge embedding at very low cost, with application to symmetry-adapted perturbation theory. Journal of Chemical Physics, 2019, 151, 031102.	3.0	17
107	Electrostatics, Charge Transfer, and the Nature of the Halideâ€“Water Hydrogen Bond. Journal of Physical Chemistry A, 2021, 125, 1243-1256.	2.5	16
108	A Simple Algorithm for Determining Orthogonal, Self-Consistent Excited-State Wave Functions for a State-Specific Hamiltonian: Application to the Optical Spectrum of the Aqueous Electron. Journal of Chemical Theory and Computation, 2011, 7, 2085-2093.	5.3	15

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109	Probing Interfacial Effects on Ionization Energies: The Surprising Banality of Anionâ€“Water Hydrogen Bonding at the Air/Water Interface. Journal of the American Chemical Society, 2021, 143, 10189-10202.	13.7	15
110	Cumulants, Extensivity, and the Connected Formulation of the Contracted SchrÃ¶dinger Equation. Advances in Chemical Physics, 2007, , 261-292.	0.3	14
111	Accuracy of finiteâ€difference harmonic frequencies in density functional theory. Journal of Computational Chemistry, 2017, 38, 1678-1684.	3.3	14
112	Natural Charge-Transfer Analysis: Eliminating Spurious Charge-Transfer States in Time-Dependent Density Functional Theory via Diabatization, with Application to Projection-Based Embedding. Journal of Chemical Theory and Computation, 2021, 17, 4195-4210.	5.3	14
113	Nonadiabatic dynamics with spin-flip vs linear-response time-dependent density functional theory: A case study for the protonated SchiffÂbase C5H6NH2+. Journal of Chemical Physics, 2021, 155, 124111.	3.0	14
114	Structure and spectroscopy of NenSHâ€,(Ãƒâ€Š2Î£+) complexes using adiabatic diffusion Monte Carlo (ADMC). Journal of Chemical Physics, 1999, 111, 9203-9212.	3.0	13
115	Intrinsically smooth discretisation of Connolly's solvent-excluded molecular surface. Molecular Physics, 2020, 118, .	1.7	13
116	Role of hemibonding in the structure and ultraviolet spectroscopy of the aqueous hydroxyl radical. Physical Chemistry Chemical Physics, 2020, 22, 27829-27844.	2.8	11
117	Using Atomic Confining Potentials for Geometry Optimization and Vibrational Frequency Calculations in Quantum-Chemical Models of Enzyme Active Sites. Journal of Physical Chemistry B, 2020, 124, 1137-1147.	2.6	11
118	Simplified tuning of long-range corrected density functionals for use in symmetry-adapted perturbation theory. Journal of Chemical Physics, 2021, 155, 034103.	3.0	11
119	Hidden Hemibonding in the Aqueous Hydroxyl Radical. Journal of Physical Chemistry Letters, 2021, 12, 8053-8060.	4.6	11
120	Comprehensive Basis-Set Testing of Extended Symmetry-Adapted Perturbation Theory and Assessment of Mixed-Basis Combinations to Reduce Cost. Journal of Chemical Theory and Computation, 2022, 18, 2308-2330.	5.3	11
121	High harmonic spectra computed using time-dependent Kohnâ€“Sham theory with Gaussian orbitals and a complex absorbing potential. Journal of Chemical Physics, 2022, 156, .	3.0	11
122	Symbolic implementation of arbitrary-order perturbation theory using computer algebra: Application to vibrationalâ€“rotational analysis of diatomic molecules. Computers & Chemistry, 1998, 22, 169-184.	1.2	9
123	Improving Generalized Born Models by Exploiting Connections to Polarizable Continuum Models. II. Corrections for Salt Effects. Journal of Chemical Theory and Computation, 2012, 8, 4381-4392.	5.3	9
124	Detection and Correction of Delocalization Errors for Electron and Hole Polarons Using Density-Corrected DFT. Journal of Physical Chemistry Letters, 2022, 13, 5275-5284.	4.6	7
125	Doubleâ€buffered, heterogeneous CPU + GPU integral digestion algorithm for singleâ€excitation calculations involving a large number of excited states. Journal of Computational Chemistry, 2018, 39, 2173-2182.	3.3	6
126	Theoretical Approach to Evaluate the Gas-Sensing Performance of Graphene Nanoribbon/Oligothiophene Composites. ACS Omega, 2022, 7, 2260-2274.	3.5	6

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127	Response to â€œComment on â€˜Curvy-steps approach to constraint-free extended-Lagrangian ab initio molecular dynamics, using atom-centered basis functions: Convergence toward Bornâ€“Oppenheimer trajectoriesâ€™ â€•[J. Chem. Phys. 123, 027101 (2005)]. Journal of Chemical Physics, 2005, 123, 027102.	3.0	5
128	Response to â€œComment on â€˜A smooth, nonsingular, and faithful discretization scheme for polarizable continuum models: The switching/Gaussian approachâ€™â€•[J. Chem. Phys. 134, 117101 (2011)]. Journal of Chemical Physics, 2011, 134, .	3.0	5
129	Interaction Energy Analysis of Monovalent Inorganic Anions in Bulk Water Versus Air/Water Interface. Molecules, 2021, 26, 6719.	3.8	5
130	How Well Does a Solvated Octa-acid Capsule Shield the Embedded Chromophore? A Computational Analysis Based on an Anisotropic Dielectric Continuum Model. Journal of Physical Chemistry B, 2020, 124, 6998-7004.	2.6	4
131	Vibrational exciton delocalization precludes the use of infrared intensities as proxies for surfactant accumulation on aqueous surfaces. Chemical Science, 2021, 12, 8320-8332.	7.4	3
132	Renormalized ladder-type expansions for many-particle propagators. Physical Review A, 2002, 66, .	2.5	2
133	Title is missing!. , 0, , .		2
134	Ab InitioApproach to Femtosecond Stimulated Raman Spectroscopy: Investigating Vibrational Modes Probed in Excited-State Relaxation of Quaterthiophenes. Journal of Physical Chemistry A, 2020, 124, 6356-6362.	2.5	1
135	State-specific solvation for restricted active space spinâ€“flip (RAS-SF) wave functions based on the polarizable continuum formalism. Journal of Chemical Physics, 2022, 156, .	3.0	1
136	Appraisal of dispersion damping functions for the effective fragment potential method. Molecular Physics, 2023, 121, .	1.7	0