John M Herbert

List of Publications by Citations

131 papers	10,178 citations	45 h-index	99 g-index
167 ext. papers	11,445 ext. citations	5.5 avg, IF	6.76 L-index

#	Paper	IF	Citations
131	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
130	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
129	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	3.9	478
128	Simultaneous benchmarking of ground- and excited-state properties with long-range-corrected density functional theory. *Journal of Chemical Physics*, **2008**, 129, 034107	3.9	249
127	Both intra- and interstrand charge-transfer excited states in aqueous B-DNA are present at energies comparable to, or just above, the (1)pipi* excitonic bright states. *Journal of the American Chemical Society*, **2009**, 131, 3913-22	16.4	168
126	Charge-transfer excited states in a pi-stacked adenine dimer, as predicted using long-range-corrected time-dependent density functional theory. *Journal of Physical Chemistry B*, **2008**, 112, 6304-8	3.4	150
125	Time-Dependent Density-Functional Description of the (1)La State in Polycyclic Aromatic Hydrocarbons: Charge-Transfer Character in Disguise?. *Journal of Chemical Theory and Computation*, **2011**, 7, 1296-306	6.4	148
124	A generalized many-body expansion and a unified view of fragment-based methods in electronic structure theory. *Journal of Chemical Physics*, **2012**, 137, 064113	3.9	146
123	A smooth, nonsingular, and faithful discretization scheme for polarizable continuum models: the switching/Gaussian approach. *Journal of Chemical Physics*, **2010**, 133, 244111	3.9	137
122	Calculation of electron detachment energies for water cluster anions: an appraisal of electronic structure methods, with application to (H2O)20- AND (H2O)24-. *Journal of Physical Chemistry A*, **2005**, 109, 5217-29	2.8	129
121	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
120	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, 5446-64	2.8	97
119	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, 12739-54	2.8	91
118	Polarizable Continuum Reaction-Field Solvation Models Affording Smooth Potential Energy Surfaces. *Journal of Physical Chemistry Letters*, **2010**, 1, 556-561	6.4	89
117	The Hydrated Electron. *Annual Review of Physical Chemistry*, **2017**, 68, 447-472	15.7	88
116	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, 1680-90	6.4	88
115	Accelerated, energy-conserving Born-Oppenheimer molecular dynamics via Fock matrix extrapolation. *Physical Chemistry Chemical Physics*, **2005**, 7, 3269-75	3.6	88

114	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	3.6	79
113	Evidence for Singlet Fission Driven by Vibronic Coherence in Crystalline Tetracene. *Journal of Physical Chemistry Letters*, **2017**, 8, 1442-1448	6.4	75
112	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	3.9	75
111	Comment on "Does the hydrated electron occupy a cavity?". *Science*, **2011**, 331, 1387; author reply 1387	33.3	72
110	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	3.9	72
109	Accurate description of intermolecular interactions involving ions using symmetry-adapted perturbation theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 2473-86	6.4	70
108	Aiming for benchmark accuracy with the many-body expansion. *Accounts of Chemical Research*, **2014**, 47, 2828-36	24.3	69
107	Analytic derivative couplings for spin-flip configuration interaction singles and spin-flip time-dependent density functional theory. *Journal of Chemical Physics*, **2014**, 141, 064104	3.9	66
106	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, 235-52	2.8	65
105	Energy Decomposition Analysis with a Stable Charge-Transfer Term for Interpreting Intermolecular Interactions. *Journal of Chemical Theory and Computation*, **2016**, 12, 2569-82	6.4	62
104	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, 931-41	24.3	61
103	Curvy-steps approach to constraint-free extended-Lagrangian ab initio molecular dynamics, using atom-centered basis functions: convergence toward Born-Oppenheimer trajectories. *Journal of Chemical Physics*, **2004**, 121, 11542-56	3.9	60
102	Understanding the many-body expansion for large systems. I. Precision considerations. *Journal of Chemical Physics*, **2014**, 141, 014108	3.9	59
101	Ab Initio Implementation of the Frenkel-Davydov Exciton Model: A Naturally Parallelizable Approach to Computing Collective Excitations in Crystals and Aggregates. *Journal of Chemical Theory and Computation*, **2014**, 10, 5366-76	6.4	58
100	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, 14470-83	2.8	58
99	Symmetric versus asymmetric discretization of the integral equations in polarizable continuum solvation models. *Chemical Physics Letters*, **2011**, 509, 77-87	2.5	58
98	Time-resolved infrared spectroscopy of the lowest triplet state of thymine and thymidine. *Chemical Physics*, **2008**, 347, 383-392	2.3	58
97	Charge penetration and the origin of large O-H vibrational red-shifts in hydrated-electron clusters, (H2O)n-. *Journal of the American Chemical Society*, **2006**, 128, 13932-9	16.4	57

96	Fantasy versus reality in fragment-based quantum chemistry. *Journal of Chemical Physics*, **2019**, 151, 170901	3.9	53
95	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, 14282-7	11.5	53
94	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	3.9	52
93	Accurate Intermolecular Interactions at Dramatically Reduced Cost: XPol+SAPT with Empirical Dispersion. *Journal of Physical Chemistry Letters*, **2012**, 3, 3241-3248	6.4	49
92	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, 19889-99	16.4	49
91	Optical spectroscopy of the bulk and interfacial hydrated electron from ab initio calculations. *Journal of Physical Chemistry A*, **2014**, 118, 7507-15	2.8	48
90	Rapid computation of intermolecular interactions in molecular and ionic clusters: self-consistent polarization plus symmetry-adapted perturbation theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 7679-99	3.6	48
89	Standard grids for high-precision integration of modern density functionals: SG-2 and SG-3. *Journal of Computational Chemistry*, **2017**, 38, 869-882	3.5	47
88	N-representability and variational stability in natural orbital functional theory. *Journal of Chemical Physics*, **2003**, 118, 10835-10846	3.9	46
87	Understanding the many-body expansion for large systems. II. Accuracy considerations. *Journal of Chemical Physics*, **2016**, 144, 164105	3.9	46
86	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	3.6	45
85	Polarization-bound quasi-continuum states are responsible for the "blue tail" in the optical absorption spectrum of the aqueous electron. *Journal of the American Chemical Society*, **2010**, 132, 10000-2	16.4	45
84	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	7	45
83	Many-Body Expansion with Overlapping Fragments: Analysis of Two Approaches. *Journal of Chemical Theory and Computation*, **2013**, 9, 1408-16	6.4	44
82	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	3.9	44
81	Analytic derivative couplings in time-dependent density functional theory: Quadratic response theory versus pseudo-wavefunction approach. *Journal of Chemical Physics*, **2015**, 142, 064109	3.9	43
80	Pair-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, 572-84	6.4	42
79	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	3.9	42

78	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, 10879-86	16.4	42
77	Comparison of the Marcus and Pekar partitions in the context of non-equilibrium, polarizable-continuum solvation models. *Journal of Chemical Physics*, **2015**, 143, 204104	3.9	40
76	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	3.9	40
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74	Stabilization and rovibronic spectra of the T-shaped and linear ground-state conformers of a weakly bound rare-gas-homonuclear dihalogen complex: He...Br2. *Journal of Chemical Physics*, **2005**, 123, 104312	3.9	39
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72	Ab Initio Investigation of Electron Detachment in Dicarboxylate Dianions. *Journal of Physical Chemistry A*, **2000**, 104, 11786-11795	2.8	38
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69	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	6.4	35
68	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, 2674-80	6.4	34
67	Breakdown of the single-exchange approximation in third-order symmetry-adapted perturbation theory. *Journal of Physical Chemistry A*, **2012**, 116, 3042-7	2.8	33
66	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	3.9	33
65	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, 4390-6	6.4	31
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62	Dielectric continuum methods for quantum chemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1519	7.9	31
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58	Energy-Screened Many-Body Expansion: A Practical Yet Accurate Fragmentation Method for Quantum Chemistry. *Journal of Chemical Theory and Computation*, **2020**, 16, 475-487	6.4	27
57	Extensivity and the contracted Schr□dinger equation. *Journal of Chemical Physics*, **2002**, 117, 7464-7471	3.9	25
56	Electrostatics does not dictate the slip-stacked arrangement of aromatic □□ interactions. *Chemical Science*, **2020**, 11, 6758-6765	9.4	24
55	The Quantum Chemistry of Loosely-Bound Electrons. *Reviews in Computational Chemistry*, **2015**, 391-517		24
54	Symmetry-adapted perturbation theory with Kohn-Sham orbitals using non-empirically tuned, long-range-corrected density functionals. *Journal of Chemical Physics*, **2014**, 140, 044108	3.9	24
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49	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	3.9	20
48	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	3.9	20
47	Approaching the complete-basis limit with a truncated many-body expansion. *Journal of Chemical Physics*, **2013**, 139, 224102	3.9	20
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40	Reinterpreting stacking. *Physical Chemistry Chemical Physics*, **2020**, 22, 24870-24886	3.6	18
39	Investigation of the Resonance Raman Spectrum of the Hydrated Electron. *Journal of Physical Chemistry B*, **2019**, 123, 8074-8085	3.4	17
38	Interaction of Graphene Quantum Dots with Oligothiophene: A Comprehensive Theoretical Study. *Journal of Physical Chemistry C*, **2019**, 123, 29556-29570	3.8	17
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33	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, 4338-46	6.4	13
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31	Cumulants, Extensivity, and the Connected Formulation of the Contracted Schrödinger Equation. *Advances in Chemical Physics*, **2007**, 261-292		13
30	Structure and spectroscopy of NenSH (2) complexes using adiabatic diffusion Monte Carlo (ADMC). *Journal of Chemical Physics*, **1999**, 111, 9203-9212	3.9	13
29	A Simple Correction for Nonadditive Dispersion within Extended Symmetry-Adapted Perturbation Theory (XSAPT). *Journal of Chemical Theory and Computation*, **2018**, 14, 5128-5142	6.4	13
28	Self-consistent charge embedding at very low cost, with application to symmetry-adapted perturbation theory. *Journal of Chemical Physics*, **2019**, 151, 031102	3.9	12
27	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	3.8	12
26	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, 2085-93	6.4	12
25	Accuracy of finite-difference harmonic frequencies in density functional theory. *Journal of Computational Chemistry*, **2017**, 38, 1678-1684	3.5	10

24	Charge Separation and Charge Transfer in the Low-Lying Excited States of Pentacene. *Journal of Physical Chemistry C*, **2020**, 124, 24653-24666	3.8	10
23	Intrinsically smooth discretisation of Connolly's solvent-excluded molecular surface. *Molecular Physics*, **2020**, 118, e1644384	1.7	9
22	What Is the Price of Open-Source Software?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2751-4	6.4	8
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20	Probing Interfacial Effects on Ionization Energies: The Surprising Banality of Anion-Water Hydrogen Bonding at the Air/Water Interface. *Journal of the American Chemical Society*, **2021**, 143, 10189-10202	16.4	8
19	Electrostatics, Charge Transfer, and the Nature of the Halide-Water Hydrogen Bond. *Journal of Physical Chemistry A*, **2021**, 125, 1243-1256	2.8	8
18	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	3.4	7
17	Symbolic implementation of arbitrary-order perturbation theory using computer algebra: Application to vibrational–rotational analysis of diatomic molecules. *Computers & Chemistry*, **1998**, 22, 169-184		6
16	Role of hemibonding in the structure and ultraviolet spectroscopy of the aqueous hydroxyl radical. *Physical Chemistry Chemical Physics*, **2020**, 22, 27829-27844	3.6	6
15	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	6.4	6
14	Simplified tuning of long-range corrected density functionals for use in symmetry-adapted perturbation theory. *Journal of Chemical Physics*, **2021**, 155, 034103	3.9	6
13	Predicting and Understanding Non-Covalent Interactions Using Novel Forms of Symmetry-Adapted Perturbation Theory. *Accounts of Chemical Research*, **2021**, 54, 3679-3690	24.3	6
12	Response to "Comment on 'A smooth, nonsingular, and faithful discretization scheme for polarizable continuum models: The switching/Gaussian approach' [J. Chem. Phys. 134, 117101 (2011)]. *Journal of Chemical Physics*, **2011**, 134, 117102	3.9	5
11	Response to "Comment on 'Curvy-steps approach to constraint-free extended-Lagrangian ab initio molecular dynamics, using atom-centered basis functions: Convergence toward Born–Oppenheimer trajectories'" [J. Chem. Phys. 123, 027101 (2005)]. *Journal of Chemical Physics*, **2005**, 123, 027102	3.9	5
10	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	3.4	4
9	Neat, Simple, and Wrong: Debunking Electrostatic Fallacies Regarding Noncovalent Interactions. *Journal of Physical Chemistry A*, **2021**, 125, 7125-7137	2.8	3
8	Renormalized ladder-type expansions for many-particle propagators. *Physical Review A*, **2002**, 66,	2.6	2
7	Broadband X-Ray Absorption Spectra from Time-Dependent Kohn-Sham Calculations		2

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5	Double-buffered, heterogeneous CPU + GPU integral digestion algorithm for single-excitation calculations involving a large number of excited states. *Journal of Computational Chemistry*, **2018**, 39, 2173-2182	3.5	2
4	Approach to Femtosecond Stimulated Raman Spectroscopy: Investigating Vibrational Modes Probed in Excited-State Relaxation of Quaterthiophenes. *Journal of Physical Chemistry A*, **2020**, 124, 6356-6362	2.8	1
3	Hidden Hemibonding in the Aqueous Hydroxyl Radical. *Journal of Physical Chemistry Letters*, **2021**, 12, 8053-8060	6.4	1
2	Nonadiabatic dynamics with spin-flip vs linear-response time-dependent density functional theory: A case study for the protonated Schiff base CHNH. *Journal of Chemical Physics*, **2021**, 155, 124111	3.9	1
1	Theoretical Approach to Evaluate the Gas-Sensing Performance of Graphene Nanoribbon/Oligothiophene Composites.. *ACS Omega*, **2022**, 7, 2260-2274	3.9	0