Daniel M Chipman

List of Publications by Year
in descending order

116 papers	9,786 citations	87888 38 h-index	36028 97 g-index
118 all docs	118 docs citations	118 times ranked	9164 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	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	47.7	560
4	Reaction field treatment of charge penetration. Journal of Chemical Physics, 2000, 112, 5558-5565.	3.0	254
5	Computation of pKafrom Dielectric Continuum Theory. Journal of Physical Chemistry A, 2002, 106, 7413-7422.	2.5	204
6	Volume polarization in reaction field theory. Journal of Chemical Physics, 1998, 108, 177-192.	3.0	132
7	Preferred orientation of imidazole ligands in metalloporphyrins. Journal of the American Chemical Society, 1986, 108, 1163-1167.	13.7	129
8	Gaussian basis sets for calculation of spin densities in first-row atoms. Theoretica Chimica Acta, 1989, 76, 73-84.	0.8	126
9	The spin polarization model for hyperfine coupling constants. Theoretica Chimica Acta, 1992, 82, 93-115.	0.8	120
10	Perturbation theories for the calculation of molecular interaction energies. I. General formalism. Journal of Chemical Physics, 1973, 59, 2830-2837.	3.0	116
11	Charge penetration in dielectric models of solvation. Journal of Chemical Physics, 1997, 106, 10194-10206.	3.0	111
12	Cavity size in reaction field theory. Journal of Chemical Physics, 1998, 109, 10543-10558.	3.0	105
13	Comparison of solvent reaction field representations. Theoretical Chemistry Accounts, 2002, 107, 80-89.	1.4	91
14	Theoretical study of the properties of methyl radical. Journal of Chemical Physics, 1983, 78, 3112-3132.	3.0	88
15	Calculation of spin densities in diatomic firstâ€row hydrides. Journal of Chemical Physics, 1989, 91, 5455-5465.	3.0	87
16	Reaction field effects on nitrogen shielding. Journal of Chemical Physics, 1999, 110, 1611-1622.	3.0	86
17	Structure and fundamental vibrations of phenoxyl radical. Journal of Chemical Physics, 1994, 100, 5023-5035.	3.0	83
18	Torsional effects on the one-bond 13C-13C spin coupling constant in ethylene glycol: insights into the behavior of 1JCC in carbohydrates. Journal of the American Chemical Society, 1993, 115, 10863-10870.	13.7	71

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19	Excited electronic states of small water clusters. Journal of Chemical Physics, 2005, 122, 044111.	3.0	69
20	Simulation of volume polarization in reaction field theory. Journal of Chemical Physics, 1999, 110, 8012-8018.	3.0	67
21	Perturbation theories for the calculation of molecular interaction energies. II. Application to H2+. Journal of Chemical Physics, 1973, 59, 2838-2857.	3.0	64
22	Structures and fundamental vibrations of p-benzoquinone and p-benzosemiquinone radical anion from ab initio calculations. The Journal of Physical Chemistry, 1986, 90, 5557-5560.	2.9	64
23	Resonance Raman spectra and structure of phenylthiyl radical. The Journal of Physical Chemistry, 1992, 96, 5344-5350.	2.9	61
24	Theoretical study on the electron affinity of the water dimer. The Journal of Physical Chemistry, 1979, 83, 1657-1662.	2.9	59
25	Ab initio calculation of spin densities in hydrocarbon radicals. Journal of Chemical Physics, 1979, 71, 761-768.	3.0	55
26	Molecular orbital studies of hyperfine coupling constants in the H2CN and H(HO)CN radicals. The Journal of Physical Chemistry, 1991, 95, 4702-4708.	2.9	50
27	Behavior of electronic wave functions near cusps. Journal of Chemical Physics, 1996, 104, 9908-9912.	3.0	50
28	Probing Silver Nanoparticles During Catalytic H2 Evolution. Journal of the American Chemical Society, 2008, 130, 7067-7076.	13.7	49
29	Resonance Raman and molecular orbital studies of the effects of deuteration on the vibrational structure of the p-benzosemiquinone radical anion. The Journal of Physical Chemistry, 1983, 87, 5357-5361.	2.9	48
30	Carbon-13 hyperfine constants of allyl radical. The Journal of Physical Chemistry, 1988, 92, 3778-3781.	2.9	47
31	Stretching of hydrogen-bonded OH in the lowest singlet excited electronic state of water dimer. Journal of Chemical Physics, 2006, 124, 044305.	3.0	47
32	New formulation and implementation for volume polarization in dielectric continuum theory. Journal of Chemical Physics, 2006, 124, 224111.	3.0	46
33	Hydration Energy from a Composite Method for Implicit Representation of Solvent. Journal of Chemical Theory and Computation, 2014, 10, 211-219.	5.3	46
34	Implementation of solvent reaction fields for electronic structure. Theoretical Chemistry Accounts, 2002, 107, 90-102.	1.4	45
35	The solvation reaction field for a hydrogen atom in a dielectric continuum. Journal of Chemical Physics, 1996, 104, 3276-3289.	3.0	42
36	Theoretical dipole moment derivatives and force constants for HCN. Journal of Chemical Physics, 1978, 69, 1425-1428.	3.0	40

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37	Energy correction to simulation of volume polarization in reaction field theory. Journal of Chemical Physics, 2002, 116, 10129-10138.	3.0	40
38	Theoretical study of the reactions of ethene with diimide species. Journal of the American Chemical Society, 1979, 101, 2290-2296.	13.7	39
39	Absorption Spectrum of OH Radical in Water. Journal of Physical Chemistry A, 2008, 112, 13372-13381.	2.5	38
40	Hemibonding between Hydroxyl Radical and Water. Journal of Physical Chemistry A, 2011, 115, 1161-1171.	2.5	37
41	Effect of molecular geometry on the electron affinity of water. The Journal of Physical Chemistry, 1978, 82, 1080-1083.	2.9	35
42	Theoretical study of the cyclopropenyl radical. Journal of the American Chemical Society, 1984, 106, 6236-6242.	13.7	34
43	Furanose ring conformation: the application of ab initio molecular orbital calculations to the structure and dynamics of erythrofuranose and threofuranose rings. Journal of the American Chemical Society, 1987, 109, 5297-5303.	13.7	34
44	Anion electric field is related to hydration energy. Journal of Chemical Physics, 2003, 118, 9937-9942.	3.0	34
45	Spin densities of first-row atoms calculated from polarization wave functions with accurate numerical methods. Physical Review A, 1989, 39, 475-480.	2.5	32
46	Hydrogen-Bonding Effects on Free-Radical Properties. Journal of Physical Chemistry A, 2000, 104, 11816-11821.	2.5	31
47	Theoretical study of hyperfine coupling constants in ethyl radical. Journal of Chemical Physics, 1991, 94, 6632-6637.	3.0	30
48	New Implicit Solvation Models for Dispersion and Exchange Energies. Journal of Physical Chemistry A, 2013, 117, 5812-5820.	2.5	29
49	Effects of bridging hydrogens on metal-metal bonds. 1. Geometrical comparison of Fe3(.mu.-H)3(CO)9(.mu.3-CMe), Co3(CO)9(.mu.3-CMe), and model compounds. Inorganic Chemistry, 1982, 21, 3197-3202.	4.0	28
50	Carbon-13 hyperfine constants of methyleneamidogen, hydroxymethyleneamidogen and aminooxomethyl radicals. The Journal of Physical Chemistry, 1988, 92, 3781-3784.	2.9	28
51	Solution of the linearized Poissonâ€“Boltzmann equation. Journal of Chemical Physics, 2004, 120, 5566-5575.	3.0	28
52	New operators for electronic density calculation. I. Derivations and formal analysis. Journal of Chemical Physics, 1996, 105, 1470-1478.	3.0	27
53	Cation electric field is related to hydration energy. Journal of Chemical Physics, 2006, 124, 144507.	3.0	27
54	Accurate width and position of lowest 1S resonance in Hâ¯ calculated from realâ€valued stabilization graphs. Journal of Chemical Physics, 1987, 86, 3819-3828.	3.0	25

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55	Ab initio studies of structure and hyperfine coupling in cyclohexadienyl and hydroxycyclohexadienyl radicals. The Journal of Physical Chemistry, 1992, 96, 3294-3298.	2.9	25
56	Comment on ab initio calculation of spin densities in hydrocarbon radicals. Journal of Chemical Physics, 1983, 78, 4785-4786.	3.0	23
57	Electron affinity of hydroxyl radical. Journal of Chemical Physics, 1986, 84, 1677-1682.	3.0	23
58	Vertical electronic excitation with a dielectric continuum model of solvation including volume polarization. I. Theory. Journal of Chemical Physics, 2009, 131, 014103.	3.0	23
59	Insights into the ultraviolet spectrum of liquid water from model calculations. Journal of Chemical Physics, 2010, 132, 244307.	3.0	22
60	Field-Extremum Model for Short-Range Contributions to Hydration Free Energy. Journal of Chemical Theory and Computation, 2011, 7, 3952-3960.	5.3	22
61	Composite Method for Implicit Representation of Solvent in Dimethyl Sulfoxide and Acetonitrile. Journal of Physical Chemistry A, 2015, 119, 5173-5180.	2.5	22
62	Para phenylenediamine radical cation structure studied by resonance Raman and molecular orbital	3.0	21
63	Modeling short-range contributions to hydration energies with minimal parameterization. Chemical Physics Letters, 2011, 511, 161-165.	2.6	21
64	Localization in exchange perturbation theory. Journal of Chemical Physics, 1977, 66, 1830-1834.	3.0	20
65	New operators for electronic density calculation. II. Application to hydrogen, firstâ€row atoms, and firstâ€row diatomic hydrides. Journal of Chemical Physics, 1996, 105, 1479-1491.	3.0	20
66	Insights into the ultraviolet spectrum of liquid water from model calculations: The different roles of donor and acceptor hydrogen bonds in water pentamers. Journal of Chemical Physics, 2012, 137, 184301.	3.0	20
67	Vacuum ultraviolet spectroscopy of the lowest-lying electronic state in subcritical and supercritical water. Nature Communications, 2017, 8, 15435.	12.8	20
68	Endo hydrogens on Main Group-transition metal clusters. Theoretical analysis of the interconversion of FeHFe and EHFe interactions and deprotonation of Fe3(CO)9EHx (E = B, x = 5; E = C, x = 4). Organometallics, 1987, 6, 2405-2412.	2.3	19
69	Effect of Hydrogen Bonding on the Vibrations ofp-Benzosemiquinone Radical Anion. Journal of Physical Chemistry A, 1998, 102, 1230-1235.	2.5	19
70	Resonance Raman, electron spin resonance and molecular orbital studies of m-benzosemiquinone radical anion. The Journal of Physical Chemistry, 1986, 90, 3968-3975.	2.9	18
71	Structure and Properties ofp-Aminophenoxyl Radical. Journal of Physical Chemistry A, 1999, 103, 11181-11187.	2.5	17
72	Theoretical studies on the singlet and triplet cyclopropylidene allene system. Journal of the American Chemical Society, 1978, 100, 5272-5278.	13.7	16

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73	Are bonds bent? To what extent do bond orbitals follow nuclear motions?. Journal of the American Chemical Society, 1980, 102, 3377-3383.	13.7	16
74	Benchmarking density functionals and Gaussian basis sets for calculation of core-electron binding energies in amino acids. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	16
75	Assignment of states in the valence photoelectron spectrum of H2S. Journal of Electron Spectroscopy and Related Phenomena, 1978, 14, 323-329.	1.7	15
76	Magnetic Hyperfine Coupling Constants in Free Radicals. , 1995, , 109-138.		15
77	Boundary element methods for dielectric cavity construction and integration. Journal of Chemical Physics, 2003, 119, 10289-10297.	3.0	15
78	Solitons in polyacetylene: Magnetic hyperfine constants fromabinitiocalculations. Journal of Chemical Physics, 1991, 95, 7698-7716.	3.0	14
79	Dissociation of Ozonide in Water. Journal of Physical Chemistry A, 2000, 104, 4629-4635.	2.5	14
80	The perfectâ€pairing valence bond model for the water molecule. Journal of Chemical Physics, 1976, 65, 2556-2561.	3.0	13
81	Water from Ambient to Supercritical Conditions with the AMOEBA Model. Journal of Physical Chemistry B, 2013, 117, 5148-5155.	2.6	13
82	Hemibonding between Water Cation and Water. Journal of Physical Chemistry A, 2016, 120, 9618-9624.	2.5	13
83	Orbital hybridization. Journal of the American Chemical Society, 1977, 99, 1305-1307.	13.7	12
84	Comparison of through-space and through-bond interactions in four-membered ring systems. The Journal of Physical Chemistry, 1982, 86, 3981-3989.	2.9	12
85	Comparative study of Gaussian basis sets for calculation of core electron binding energies in first-row hydrides and glycine. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	12
86	On symmetry in the polarization expansion for intermolecular forces. Journal of Chemical Physics, 1980, 73, 5164-5167.	3.0	11
87	Spin density in first-row atoms from the Hiller-Sucher-Feinberg identity. Theoretica Chimica Acta, 1995, 91, 1-15.	0.8	11
88	Performance of density functionals for computation of core electron binding energies in first-row hydrides and glycine. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	11
89	Spin density in firstâ€row diatomic hydrides from the Hillerâ€“Sucherâ€“Feinberg identity. Journal of Chemical Physics, 1995, 103, 10058-10069.	3.0	10
90	Resonance Raman Spectrum and Structure of p-Benzodithiyl Radical Anion. The Journal of Physical Chemistry, 1995, 99, 5264-5268.	2.9	10

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91	New operators for calculation of indirect nuclear spinâ€“spin coupling constants. Journal of Chemical Physics, 1997, 107, 5488-5495.	3.0	10
92	Simulation of volume polarization for the influence of solvation on chemical shielding. Theoretical Chemistry Accounts, 2004, 111, 61-65.	1.4	10
93	Vertical electronic excitation with a dielectric continuum model of solvation including volume polarization. II. Implementation and applications. Journal of Chemical Physics, 2009, 131, 014104.	3.0	10
94	How Does Dielectric Solvation Affect the Size of an Ion?. Journal of Physical Chemistry A, 2010, 114, 12788-12793.	2.5	10
95	On optimizing the treatment of exchange perturbations. Chemical Physics Letters, 1972, 14, 293-298.	2.6	9
96	Lithium atom spin density from the Hiller-Sucher-Feinberg identity. Theoretica Chimica Acta, 1994, 88, 339-349.	0.8	9
97	Calculation of sum rule properties for H2O. Journal of Chemical Physics, 1977, 67, 2236.	3.0	8
98	Structure and Proton Reactivity of the Semiquinone Anion and Dianion of Biphenol in Water. Journal of Physical Chemistry A, 2002, 106, 8908-8916.	2.5	7
99	Comment on symmetry-adapted perturbation theories. Chemical Physics Letters, 1976, 40, 147-149.	2.6	6
100	Dissociative electron attachment to the hydrogen-bound OH in water dimer through the lowest anionic Feshbach resonance. Journal of Chemical Physics, 2007, 127, 194309.	3.0	6
101	Hydrogen Atom in Water from Ambient to High Temperatures. Journal of Physical Chemistry B, 2013, 117, 16530-16541.	2.6	6
102	The Valence Bond Orbital Model as an Interpretive Framework for Understanding Electronic Structure. Israel Journal of Chemistry, 1980, 19, 82-87.	2.3	5
103	Theoretical Identification of a Radical Produced by Radiolysis of Uracil. Radiation Research, 1981, 85, 257.	1.5	5
104	Partial widths of resonances by analytic continuation from real eigenvalues. Chemical Physics Letters, 1990, 167, 246-251.	2.6	5
105	Structures and Energetics of Hydrated Oxygen Anion Clusters. Journal of Physical Chemistry A, 2005, 109, 7418-7428.	2.5	5
106	Accurate â€œdoubly-occupied orbital seaâ€•approximation for the many-electron valence bond wavefunction. Chemical Physics Letters, 1974, 26, 593-595.	2.6	4
107	Thermal transformations of cis-1,2-dibenzoylalkenes. Journal of Organic Chemistry, 1980, 45, 3187-3191.	3.2	4
108	Electron impact on N2/CH4 mixtures in He dropletsâ€”probing chemistry in Titan's atmosphere. RSC Advances, 2012, 2, 10492.	3.6	4

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109	Ionization potentials of water from valence bond and molecular orbital wave functions. Journal of the American Chemical Society, 1978, 100, 2650-2654.	13.7	3
110	Exchange perturbation theory for electron scattering. Elastic scattering from hydrogen atoms. Physical Review A, 1980, 21, 1443-1452.	2.5	3
111	Interaction of nonbonding orbitals in 1,3-cyclobutanedione systems. The Journal of Physical Chemistry, 1982, 86, 3990-3992.	2.9	2
112	Monocarbon cationic cluster yields from N2/CH4 mixtures embedded in He nanodroplets and their calculated binding energies. Journal of Chemical Physics, 2014, 140, 034316.	3.0	2
113	Calculation of partial widths for autoionization of the 1P (3s3p) resonance state of helium. Journal of Chemical Physics, 1990, 93, 1785-1790.	3.0	1
114	Failure of molecular dynamics to provide appropriate structures for quantum mechanical description of the aqueous chloride ion charge-transfer-to-solvent ultraviolet spectrum. Physical Chemistry Chemical Physics, 2021, 23, 9109-9120.	2.8	1
115	Perturbation approach to a molecular orbital theory of interaction energies. The Journal of Physical Chemistry, 1982, 86, 1141-1146.	2.9	0
116	The Numerical Computation of Two Transcendental Functions Related to the Exponential Integral. Mathematics of Computation, 1972, 26, 241.	2.1	0