

Daniel M Chipman

List of Publications by Year in descending order

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116
papers

9,786
citations

87888

38
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36028

97
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118
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118
docs citations

118
times ranked

9164
citing authors

#	ARTICLE	IF	CITATIONS
1	Failure of molecular dynamics to provide appropriate structures for quantum mechanical description of the aqueous chloride ion charge-transfer-to-solvent ultraviolet spectrum. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9109-9120.	2.8	1
2	Vacuum ultraviolet spectroscopy of the lowest-lying electronic state in subcritical and supercritical water. <i>Nature Communications</i> , 2017, 8, 15435.	12.8	20
3	Benchmarking density functionals and Gaussian basis sets for calculation of core-electron binding energies in amino acids. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	16
4	Hemibonding between Water Cation and Water. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9618-9624.	2.5	13
5	Composite Method for Implicit Representation of Solvent in Dimethyl Sulfoxide and Acetonitrile. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5173-5180.	2.5	22
6	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	1.7	2,561
7	Monocarbon cationic cluster yields from N ₂ /CH ₄ mixtures embedded in He nanodroplets and their calculated binding energies. <i>Journal of Chemical Physics</i> , 2014, 140, 034316.	3.0	2
8	Hydration Energy from a Composite Method for Implicit Representation of Solvent. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 211-219.	5.3	46
9	Comparative study of Gaussian basis sets for calculation of core electron binding energies in first-row hydrides and glycine. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	12
10	Performance of density functionals for computation of core electron binding energies in first-row hydrides and glycine. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	11
11	Water from Ambient to Supercritical Conditions with the AMOEBA Model. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5148-5155.	2.6	13
12	New Implicit Solvation Models for Dispersion and Exchange Energies. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5812-5820.	2.5	29
13	Hydrogen Atom in Water from Ambient to High Temperatures. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16530-16541.	2.6	6
14	Electron impact on N ₂ /CH ₄ mixtures in He droplets—probing chemistry in Titan's atmosphere. <i>RSC Advances</i> , 2012, 2, 10492.	3.6	4
15	Insights into the ultraviolet spectrum of liquid water from model calculations: The different roles of donor and acceptor hydrogen bonds in water pentamers. <i>Journal of Chemical Physics</i> , 2012, 137, 184301.	3.0	20
16	Field-Extremum Model for Short-Range Contributions to Hydration Free Energy. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3952-3960.	5.3	22
17	Hemibonding between Hydroxyl Radical and Water. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1161-1171.	2.5	37
18	Modeling short-range contributions to hydration energies with minimal parameterization. <i>Chemical Physics Letters</i> , 2011, 511, 161-165.	2.6	21

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19	Insights into the ultraviolet spectrum of liquid water from model calculations. <i>Journal of Chemical Physics</i> , 2010, 132, 244307.	3.0	22
20	How Does Dielectric Solvation Affect the Size of an Ion?. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12788-12793.	2.5	10
21	Vertical electronic excitation with a dielectric continuum model of solvation including volume polarization. II. Implementation and applications. <i>Journal of Chemical Physics</i> , 2009, 131, 014104.	3.0	10
22	Vertical electronic excitation with a dielectric continuum model of solvation including volume polarization. I. Theory. <i>Journal of Chemical Physics</i> , 2009, 131, 014103.	3.0	23
23	Absorption Spectrum of OH Radical in Water. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13372-13381.	2.5	38
24	Probing Silver Nanoparticles During Catalytic H ₂ Evolution. <i>Journal of the American Chemical Society</i> , 2008, 130, 7067-7076.	13.7	49
25	Dissociative electron attachment to the hydrogen-bound OH in water dimer through the lowest anionic Feshbach resonance. <i>Journal of Chemical Physics</i> , 2007, 127, 194309.	3.0	6
26	New formulation and implementation for volume polarization in dielectric continuum theory. <i>Journal of Chemical Physics</i> , 2006, 124, 224111.	3.0	46
27	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3172-3191.	2.8	2,597
28	Stretching of hydrogen-bonded OH in the lowest singlet excited electronic state of water dimer. <i>Journal of Chemical Physics</i> , 2006, 124, 044305.	3.0	47
29	Cation electric field is related to hydration energy. <i>Journal of Chemical Physics</i> , 2006, 124, 144507.	3.0	27
30	Structures and Energetics of Hydrated Oxygen Anion Clusters. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7418-7428.	2.5	5
31	Role of Water in Electron-Initiated Processes and Radical Chemistry: Issues and Scientific Advances. <i>Chemical Reviews</i> , 2005, 105, 355-390.	47.7	560
32	Excited electronic states of small water clusters. <i>Journal of Chemical Physics</i> , 2005, 122, 044111.	3.0	69
33	Solution of the linearized Poisson-Boltzmann equation. <i>Journal of Chemical Physics</i> , 2004, 120, 5566-5575.	3.0	28
34	Simulation of volume polarization for the influence of solvation on chemical shielding. <i>Theoretical Chemistry Accounts</i> , 2004, 111, 61-65.	1.4	10
35	Anion electric field is related to hydration energy. <i>Journal of Chemical Physics</i> , 2003, 118, 9937-9942.	3.0	34
36	Boundary element methods for dielectric cavity construction and integration. <i>Journal of Chemical Physics</i> , 2003, 119, 10289-10297.	3.0	15

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37	Energy correction to simulation of volume polarization in reaction field theory. <i>Journal of Chemical Physics</i> , 2002, 116, 10129-10138.	3.0	40
38	Computation of pK _a from Dielectric Continuum Theory. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7413-7422.	2.5	204
39	Structure and Proton Reactivity of the Semiquinone Anion and Dianion of Biphenol in Water. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8908-8916.	2.5	7
40	Comparison of solvent reaction field representations. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 80-89.	1.4	91
41	Implementation of solvent reaction fields for electronic structure. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 90-102.	1.4	45
42	Reaction field treatment of charge penetration. <i>Journal of Chemical Physics</i> , 2000, 112, 5558-5565.	3.0	254
43	Dissociation of Ozonide in Water. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4629-4635.	2.5	14
44	Hydrogen-Bonding Effects on Free-Radical Properties. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11816-11821.	2.5	31
45	Simulation of volume polarization in reaction field theory. <i>Journal of Chemical Physics</i> , 1999, 110, 8012-8018.	3.0	67
46	Reaction field effects on nitrogen shielding. <i>Journal of Chemical Physics</i> , 1999, 110, 1611-1622.	3.0	86
47	Structure and Properties of p-Aminophenoxy Radical. <i>Journal of Physical Chemistry A</i> , 1999, 103, 11181-11187.	2.5	17
48	Cavity size in reaction field theory. <i>Journal of Chemical Physics</i> , 1998, 109, 10543-10558.	3.0	105
49	Effect of Hydrogen Bonding on the Vibrations of p-Benzosemiquinone Radical Anion. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1230-1235.	2.5	19
50	Volume polarization in reaction field theory. <i>Journal of Chemical Physics</i> , 1998, 108, 177-192.	3.0	132
51	Charge penetration in dielectric models of solvation. <i>Journal of Chemical Physics</i> , 1997, 106, 10194-10206.	3.0	111
52	New operators for calculation of indirect nuclear spin-spin coupling constants. <i>Journal of Chemical Physics</i> , 1997, 107, 5488-5495.	3.0	10
53	Behavior of electronic wave functions near cusps. <i>Journal of Chemical Physics</i> , 1996, 104, 9908-9912.	3.0	50
54	New operators for electronic density calculation. II. Application to hydrogen, first-row atoms, and first-row diatomic hydrides. <i>Journal of Chemical Physics</i> , 1996, 105, 1479-1491.	3.0	20

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55	New operators for electronic density calculation. I. Derivations and formal analysis. Journal of Chemical Physics, 1996, 105, 1470-1478.	3.0	27
56	The solvation reaction field for a hydrogen atom in a dielectric continuum. Journal of Chemical Physics, 1996, 104, 3276-3289.	3.0	42
57	Spin density in first-row diatomic hydrides from the Hiller-Sucher-Feinberg identity. Journal of Chemical Physics, 1995, 103, 10058-10069.	3.0	10
58	Resonance Raman Spectrum and Structure of p-Benzodithiyl Radical Anion. The Journal of Physical Chemistry, 1995, 99, 5264-5268.	2.9	10
59	Magnetic Hyperfine Coupling Constants in Free Radicals. , 1995, , 109-138.		15
60	Spin density in first-row atoms from the Hiller-Sucher-Feinberg identity. Theoretica Chimica Acta, 1995, 91, 1-15.	0.8	11
61	Lithium atom spin density from the Hiller-Sucher-Feinberg identity. Theoretica Chimica Acta, 1994, 88, 339-349.	0.8	9
62	Structure and fundamental vibrations of phenoxyl radical. Journal of Chemical Physics, 1994, 100, 5023-5035.	3.0	83
63	Torsional effects on the one-bond ¹³ C- ¹³ C spin coupling constant in ethylene glycol: insights into the behavior of ¹ JCC in carbohydrates. Journal of the American Chemical Society, 1993, 115, 10863-10870.	13.7	71
64	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
65	Resonance Raman spectra and structure of phenylthiyl radical. The Journal of Physical Chemistry, 1992, 96, 5344-5350.	2.9	61
66	Para phenylenediamine radical cation structure studied by resonance Raman and molecular orbital	3.0	21
67	The spin polarization model for hyperfine coupling constants. Theoretica Chimica Acta, 1992, 82, 93-115.	0.8	120
68	Theoretical study of hyperfine coupling constants in ethyl radical. Journal of Chemical Physics, 1991, 94, 6632-6637.	3.0	30
69	Solitons in polyacetylene: Magnetic hyperfine constants from ab initio calculations. Journal of Chemical Physics, 1991, 95, 7698-7716.	3.0	14
70	Molecular orbital studies of hyperfine coupling constants in the H ₂ CN and H(HO)CN radicals. The Journal of Physical Chemistry, 1991, 95, 4702-4708.	2.9	50
71	Partial widths of resonances by analytic continuation from real eigenvalues. Chemical Physics Letters, 1990, 167, 246-251.	2.6	5
72	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

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73	Calculation of spin densities in diatomic first-row hydrides. <i>Journal of Chemical Physics</i> , 1989, 91, 5455-5465.	3.0	87
74	Spin densities of first-row atoms calculated from polarization wave functions with accurate numerical methods. <i>Physical Review A</i> , 1989, 39, 475-480.	2.5	32
75	Gaussian basis sets for calculation of spin densities in first-row atoms. <i>Theoretica Chimica Acta</i> , 1989, 76, 73-84.	0.8	126
76	Carbon-13 hyperfine constants of allyl radical. <i>The Journal of Physical Chemistry</i> , 1988, 92, 3778-3781.	2.9	47
77	Carbon-13 hyperfine constants of methyleneamidogen, hydroxymethyleneamidogen and aminooxomethyl radicals. <i>The Journal of Physical Chemistry</i> , 1988, 92, 3781-3784.	2.9	28
78	Accurate width and position of lowest 1S resonance in H $\dot{\text{a}}$ calculated from real-valued stabilization graphs. <i>Journal of Chemical Physics</i> , 1987, 86, 3819-3828.	3.0	25
79	Furanose ring conformation: the application of ab initio molecular orbital calculations to the structure and dynamics of erythrofuranose and threofuranose rings. <i>Journal of the American Chemical Society</i> , 1987, 109, 5297-5303.	13.7	34
80	Endo hydrogens on Main Group-transition metal clusters. Theoretical analysis of the interconversion of FeHFe and EHFe interactions and deprotonation of Fe ₃ (CO) ₉ EH _x (E = B, x = 5; E = C, x = 4). <i>Organometallics</i> , 1987, 6, 2405-2412.	2.3	19
81	Resonance Raman, electron spin resonance and molecular orbital studies of m-benzosemiquinone radical anion. <i>The Journal of Physical Chemistry</i> , 1986, 90, 3968-3975.	2.9	18
82	Preferred orientation of imidazole ligands in metalloporphyrins. <i>Journal of the American Chemical Society</i> , 1986, 108, 1163-1167.	13.7	129
83	Structures and fundamental vibrations of p-benzoquinone and p-benzosemiquinone radical anion from ab initio calculations. <i>The Journal of Physical Chemistry</i> , 1986, 90, 5557-5560.	2.9	64
84	Electron affinity of hydroxyl radical. <i>Journal of Chemical Physics</i> , 1986, 84, 1677-1682.	3.0	23
85	Theoretical study of the cyclopropenyl radical. <i>Journal of the American Chemical Society</i> , 1984, 106, 6236-6242.	13.7	34
86	Resonance Raman and molecular orbital studies of the effects of deuteration on the vibrational structure of the p-benzosemiquinone radical anion. <i>The Journal of Physical Chemistry</i> , 1983, 87, 5357-5361.	2.9	48
87	Theoretical study of the properties of methyl radical. <i>Journal of Chemical Physics</i> , 1983, 78, 3112-3132.	3.0	88
88	Comment on ab initio calculation of spin densities in hydrocarbon radicals. <i>Journal of Chemical Physics</i> , 1983, 78, 4785-4786.	3.0	23
89	Perturbation approach to a molecular orbital theory of interaction energies. <i>The Journal of Physical Chemistry</i> , 1982, 86, 1141-1146.	2.9	0
90	Interaction of nonbonding orbitals in 1,3-cyclobutanedione systems. <i>The Journal of Physical Chemistry</i> , 1982, 86, 3990-3992.	2.9	2

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91	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
92	Effects of bridging hydrogens on metal-metal bonds. 1. Geometrical comparison of $\text{Fe}_3(\mu\text{-H})_3(\text{CO})_9(\mu\text{-}3\text{-CMe})$, $\text{Co}_3(\text{CO})_9(\mu\text{-}3\text{-CMe})$, and model compounds. Inorganic Chemistry, 1982, 21, 3197-3202.	4.0	28
93	Theoretical Identification of a Radical Produced by Radiolysis of Uracil. Radiation Research, 1981, 85, 257.	1.5	5
94	Thermal transformations of cis-1,2-dibenzoylalkenes. Journal of Organic Chemistry, 1980, 45, 3187-3191.	3.2	4
95	On symmetry in the polarization expansion for intermolecular forces. Journal of Chemical Physics, 1980, 73, 5164-5167.	3.0	11
96	Exchange perturbation theory for electron scattering. Elastic scattering from hydrogen atoms. Physical Review A, 1980, 21, 1443-1452.	2.5	3
97	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
98	The Valence Bond Orbital Model as an Interpretive Framework for Understanding Electronic Structure. Israel Journal of Chemistry, 1980, 19, 82-87.	2.3	5
99	Theoretical study of the reactions of ethene with diimide species. Journal of the American Chemical Society, 1979, 101, 2290-2296.	13.7	39
100	Theoretical study on the electron affinity of the water dimer. The Journal of Physical Chemistry, 1979, 83, 1657-1662.	2.9	59
101	Ab initio calculation of spin densities in hydrocarbon radicals. Journal of Chemical Physics, 1979, 71, 761-768.	3.0	55
102	Assignment of states in the valence photoelectron spectrum of H ₂ S. Journal of Electron Spectroscopy and Related Phenomena, 1978, 14, 323-329.	1.7	15
103	Theoretical studies on the singlet and triplet cyclopropylidene allene system. Journal of the American Chemical Society, 1978, 100, 5272-5278.	13.7	16
104	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
105	Effect of molecular geometry on the electron affinity of water. The Journal of Physical Chemistry, 1978, 82, 1080-1083.	2.9	35
106	Theoretical dipole moment derivatives and force constants for HCN. Journal of Chemical Physics, 1978, 69, 1425-1428.	3.0	40
107	Calculation of sum rule properties for H ₂ O. Journal of Chemical Physics, 1977, 67, 2236.	3.0	8
108	Localization in exchange perturbation theory. Journal of Chemical Physics, 1977, 66, 1830-1834.	3.0	20

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109	Orbital hybridization. Journal of the American Chemical Society, 1977, 99, 1305-1307.	13.7	12
110	Comment on symmetry-adapted perturbation theories. Chemical Physics Letters, 1976, 40, 147-149.	2.6	6
111	The perfect σ -pairing valence bond model for the water molecule. Journal of Chemical Physics, 1976, 65, 2556-2561.	3.0	13
112	Accurate σ -doubly-occupied orbital sea σ -approximation for the many-electron valence bond wavefunction. Chemical Physics Letters, 1974, 26, 593-595.	2.6	4
113	Perturbation theories for the calculation of molecular interaction energies. I. General formalism. Journal of Chemical Physics, 1973, 59, 2830-2837.	3.0	116
114	Perturbation theories for the calculation of molecular interaction energies. II. Application to H ₂ ⁺ . Journal of Chemical Physics, 1973, 59, 2838-2857.	3.0	64
115	On optimizing the treatment of exchange perturbations. Chemical Physics Letters, 1972, 14, 293-298.	2.6	9
116	The Numerical Computation of Two Transcendental Functions Related to the Exponential Integral. Mathematics of Computation, 1972, 26, 241.	2.1	0