Peter M W Gill

List of Publications by Year
in descending order

189 papers	18,818 citations	34105 52 h-index	11939 134 g-index
190 all docs	190 docs citations	190 times ranked	12121 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	The performance of a family of density functional methods. Journal of Chemical Physics, 1993, 98, 5612-5626.	3.0	1,809
4	The performance of the Beckeâ€"Leeâ€"Yangâ€"Parr (Bâ€"LYP) density functional theory with various basis sets. Chemical Physics Letters, 1992, 197, 499-505.	2.6	875
5	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	3.3	617
6	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
7	A standard grid for density functional calculations. Chemical Physics Letters, 1993, 209, 506-512.	2.6	438
8	Kohnâ€"Sham density-functional theory within a finite basis set. Chemical Physics Letters, 1992, 199, 557-560.	2.6	437
9	Self-Consistent Field Calculations of Excited States Using the Maximum Overlap Method (MOM). Journal of Physical Chemistry A, 2008, 112, 13164-13171.	2.5	435
10	The continuous fast multipole method. Chemical Physics Letters, 1994, 230, 8-16.	2.6	370
11	A density functional study of the simplest hydrogen abstraction reaction. Effect of self-interaction correction. Chemical Physics Letters, 1994, 221, 100-108.	2.6	334
12	Linear scaling density functional calculations via the continuous fast multipole method. Chemical Physics Letters, 1996, 253, 268-278.	2.6	327
13	Qâ€Chem: an engine for innovation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 317-326.	14.6	287
14	Self-consistent-field calculations of core excited states. Journal of Chemical Physics, 2009, 130, 124308.	3.0	254
15	Spin-unrestricted character of Kohn-Sham orbitals for open-shell systems. International Journal of Quantum Chemistry, 1995, 56, 303-305.	2.0	205
16	A new gradient-corrected exchange functional. Molecular Physics, 1996, 89, 433-445.	1.7	203
17	An investigation of the performance of a hybrid of Hartree-Fock and density functional theory. International Journal of Quantum Chemistry, 1992, 44, 319-331.	2.0	200
18	Structures and stabilities of singly charged three-electron hemibonded systems and their hydrogen-bonded isomers. Journal of the American Chemical Society, 1988, 110, 4931-4941.	13.7	194

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19	Molecular integrals Over Gaussian Basis Functions. Advances in Quantum Chemistry, 1994, 25, 141-205.	0.8	192
20	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. Journal of Computational Chemistry, 2007, 28, 1485-1502.	3.3	190
21	Auxiliary basis expansions for large-scale electronic structure calculations. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6692-6697.	7.1	184
22	Coulomb-attenuated exchange energy density functionals. Molecular Physics, 1996, 88, 1005-1009.	1.7	181
23	Isomers of C20. Dramatic effect of gradient corrections in density functional theory. Chemical Physics Letters, 1993, 214, 357-361.	2.6	144
24	EDF2: A Density Functional for Predicting Molecular Vibrational Frequencies. Australian Journal of Chemistry, 2004, 57, 365.	0.9	139
25	Simple Models for Difficult Electronic Excitations. Journal of Chemical Theory and Computation, 2018, 14, 1501-1509.	5.3	133
26	The prism algorithm for two-electron integrals. International Journal of Quantum Chemistry, 1991, 40, 753-772.	2.0	129
27	Probing the Reactivity of Photoinitiators for Free Radical Polymerization:Â Time-Resolved Infrared Spectroscopic Study of Benzoyl Radicals. Journal of the American Chemical Society, 2002, 124, 14952-14958.	13.7	128
28	Preliminary results on the performance of a family of density functional methods. Journal of Chemical Physics, 1992, 97, 7846-7848.	3.0	119
29	Why does unrestricted Mo/llerâ€“Plesset perturbation theory converge so slowly for spinâ€contaminated wave functions?. Journal of Chemical Physics, 1988, 89, 7307-7314.	3.0	109
30	Stereoselective Association of Binuclear Metallacycles in Coordination Polymers. Journal of the American Chemical Society, 2003, 125, 6753-6761.	13.7	106
31	The two faces of static correlation. Journal of Chemical Physics, 2011, 134, 114111.	3.0	103
32	Deceptive convergence in mÃ¸ller-plesset perturbation energies. Chemical Physics Letters, 1986, 132, 16-22.	2.6	101
33	An algorithm for the location of branching points on reaction paths. Journal of Computational Chemistry, 1988, 9, 465-475.	3.3	98
34	The uniform electron gas. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 410-429.	14.6	98
35	Empirical density functionals. Chemical Physics Letters, 1998, 284, 6-11.	2.6	95
36	Two-electron repulsion integrals over Gaussians functions. International Journal of Quantum Chemistry, 1991, 40, 745-752.	2.0	93

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37	Efficient computation of two-electron - repulsion integrals and their nth-order derivatives using contracted Gaussian basis sets. The Journal of Physical Chemistry, 1990, 94, 5564-5572.	2.9	88
38	Isomers of C24. Density functional studies including gradient corrections. Chemical Physics Letters, 1994, 220, 385-390.	2.6	85
39	Assessment of DFT Methods for Transition Metals with the TMC151 Compilation of Data Sets and Comparison with Accuracies for Main-Group Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 3610-3622.	5.3	85
40	Two Electrons on a Hypersphere: A Quasiexactly Solvable Model. Physical Review Letters, 2009, 103, 123008.	7.8	83
41	6-311G(MC)(d,p): a second-row analogue of the 6-311G(d,p) basis set: calculated heats of formation for second-row hydrides. The Journal of Physical Chemistry, 1988, 92, 4875-4880.	2.9	78
42	The structure and stability of the O2+2 dication: a dramatic failure of MÃ¸llerâ€”Plesset perturbation theory. Chemical Physics Letters, 1991, 182, 216-224.	2.6	78
43	Chemistry without Coulomb tails. Chemical Physics Letters, 1996, 254, 329-336.	2.6	72
44	A family of attenuated Coulomb operators. Chemical Physics Letters, 1996, 261, 105-110.	2.6	69
45	Efficient calculation of short-range Coulomb energies. Journal of Computational Chemistry, 1999, 20, 921-927.	3.3	68
46	Computing molecular electrostatic potentials with the PRISM algorithm. Chemical Physics Letters, 1993, 206, 239-246.	2.6	66
47	Transformation of Î±-Tocopherol (Vitamin E) and Related Chromanol Model Compounds into Their Phenoxonium Ions by Chemical Oxidation with the Nitrosonium Cation. Journal of Organic Chemistry, 2005, 70, 10466-10473.	3.2	63
48	KWIK:â€‰ Coulomb Energies in O(N) Work. The Journal of Physical Chemistry, 1996, 100, 6272-6276.	2.9	61
49	A family of intracules, a conjecture and the electron correlation problem. Physical Chemistry Chemical Physics, 2006, 8, 15-25.	2.8	61
50	Calculating molecular vibrational spectra beyond the harmonic approximation. Theoretical Chemistry Accounts, 2008, 120, 23-35.	1.4	61
51	The role of exchange in systematic DFT errors for some organic reactions. Physical Chemistry Chemical Physics, 2009, 11, 1138.	2.8	60
52	Ground state of two electrons on a sphere. Physical Review A, 2009, 79, .	2.5	54
53	Exact Wave Functions of Two-Electron Quantum Rings. Physical Review Letters, 2012, 108, 083002.	7.8	53
54	The ACDCP model for estimating the kinetic energy release and transition structure bond length in the fragmentation of a diatomic dication. Chemical Physics Letters, 1988, 147, 213-218.	2.6	52

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55	Communication: Hartree-Fock description of excited states of H2. Journal of Chemical Physics, 2014, 141, 111104.	3.0	50
56	Modeling the potential of a charge distribution. Journal of Chemical Physics, 1992, 96, 7178-7179.	3.0	49
57	A theoretical approach to molecular conformational analysis. Journal of Molecular Structure, 1985, 126, 271-290.	3.6	48
58	Benchmark correlation energies for small molecules. Molecular Physics, 2005, 103, 763-766.	1.7	48
59	Wave functions and two-electron probability distributions of the Hookeâ€™s-law atom and helium. Physical Review A, 2003, 68, .	2.5	45
60	Two-electron distribution functions and intracules. Theoretical Chemistry Accounts, 2003, 109, 241-250.	1.4	45
61	Performance of Density Functional Theory Procedures for the Calculation of Proton-Exchange Barriers: Unusual Behavior of M06-Type Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3777-3783.	5.3	44
62	A simple yet powerful upper bound for Coulomb integrals. Chemical Physics Letters, 1994, 217, 65-68.	2.6	43
63	A rationalization of unusually late transition structures for dication fragmentations. Chemical Physics Letters, 1987, 136, 294-298.	2.6	40
64	SG-0: A small standard grid for DFT quadrature on large systems. Journal of Computational Chemistry, 2006, 27, 730-739.	3.3	40
65	Excited states of spherium. Molecular Physics, 2010, 108, 2527-2532.	1.7	40
66	Title is missing!. Australian Journal of Chemistry, 2001, 54, 661.	0.9	39
67	Radial quadrature for multiexponential integrands. Journal of Computational Chemistry, 2003, 24, 732-740.	3.3	39
68	Excitation Number: Characterizing Multiply Excited States. Journal of Chemical Theory and Computation, 2018, 14, 9-13.	5.3	39
69	Exact exchange functional for the hydrogen atom. Physical Review A, 1993, 47, 2383-2385.	2.5	37
70	How does a dication lose a proton?. Journal of the American Chemical Society, 1988, 110, 5311-5314.	13.7	36
71	A rotationally invariant procedure for density functional calculations. Chemical Physics Letters, 1994, 220, 377-384.	2.6	36
72	Electron correlation in Hookeâ€™s law atom in the high-density limit. Journal of Chemical Physics, 2005, 122, 094110.	3.0	36

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73	An ab initio study of anharmonicity and matrix effects on the hydrogen-bonded BrH:NH3 complex. Molecular Physics, 1997, 92, 429-439.	1.7	36
74	Correlation energy of two electrons in the high-density limit. Journal of Chemical Physics, 2009, 131, 241101.	3.0	35
75	Structures and stabilities of the dimer dications of first- and second-row hydrides. Journal of the American Chemical Society, 1989, 111, 4613-4622.	13.7	34
76	Extraction of Stewart Atoms from Electron Densities. The Journal of Physical Chemistry, 1996, 100, 15421-15427.	2.9	33
77	A tensor approach to two-electron matrix elements. Journal of Chemical Physics, 1997, 107, 124-131.	3.0	31
78	Resolutions of the Coulomb operator. Journal of Chemical Physics, 2008, 128, 201104.	3.0	31
79	Invariance of the Correlation Energy at High Density and Large Dimension in Two-Electron Systems. Physical Review Letters, 2010, 105, 113001.	7.8	31
80	Uniform electron gases. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	31
81	Uniform electron gases. I. Electrons on a ring. Journal of Chemical Physics, 2013, 138, 164124.	3.0	31
82	The potential energy surface for the [C2H2O]+Ë™ system: The ketene radical cation [CH2ï£¾Cï£¾O]+Ë™ and its isomers. Organic Mass Spectrometry, 1984, 19, 610-616.	1.3	30
83	Multiply-charged cations: remarkable structures and stabilities. Pure and Applied Chemistry, 1988, 60, 183-188.	1.9	30
84	Exact and approximate solutions to the one-center McMurchie-Davidson tree-search problem. International Journal of Quantum Chemistry, 1991, 40, 809-827.	2.0	30
85	Can correlation bring electrons closer together?. Molecular Physics, 2009, 107, 1089-1093.	1.7	30
86	Resolutions of the Coulomb operator: II. The Laguerre generator. Chemical Physics, 2009, 356, 86-90.	1.9	30
87	A tale of two electrons: Correlation at high density. Chemical Physics Letters, 2010, 500, 1-8.	2.6	30
88	Coulomb-attenuated exchange energy density functionals. Molecular Physics, 1996, 88, 1005-1010.	1.7	30
89	An efficient algorithm for the generation of two-electron repulsion integrals over gaussian basis functions. International Journal of Quantum Chemistry, 2009, 36, 269-280.	2.0	29
90	Computation of Coulomb and exchange radial intracule densities. Chemical Physics Letters, 1999, 313, 271-278.	2.6	28

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91	Thinking outside the box: The uniform electron gas on a hypersphere. Journal of Chemical Physics, 2011, 135, 214111.	3.0	28
92	A new expansion of the Coulomb interaction. Chemical Physics Letters, 1997, 270, 193-195.	2.6	27
93	Intracule functional models. II. Analytically integrable kernels. Journal of Chemical Physics, 2007, 127, 141103.	3.0	27
94	The efficient transformation of (m0|n0) to (ab|cd) two-electron repulsion integrals. Chemical Physics Letters, 1993, 206, 229-238.	2.6	26
95	Insights from Coulomb and exchange intracules. Computational and Theoretical Chemistry, 2000, 506, 303-312.	1.5	26
96	The role of vibrational doorway states in positron annihilation with large molecules. Nuclear Instruments & Methods in Physics Research B, 2004, 221, 30-35.	1.4	25
97	Approaching the Hartreeâ€“Fock limit by perturbative methods. Journal of Chemical Physics, 2009, 130, 231101.	3.0	25
98	The hemibonded dimer radical cation of thiirane. Journal of the American Chemical Society, 1989, 111, 2782-2785.	13.7	24
99	Efficient calculation ofp-values in linear-statistic permutation significance tests. Journal of Statistical Computation and Simulation, 2007, 77, 55-61.	1.2	24
100	Correlation energy of two electrons in a ball. Journal of Chemical Physics, 2010, 132, 234111.	3.0	24
101	The nature of electron correlation in a dissociating bond. Journal of Chemical Physics, 2011, 134, 224103.	3.0	24
102	Optimal partition of the Coulomb operator. Physical Review A, 1997, 55, 3233-3235.	2.5	23
103	Parallelization of SCF calculations within Q-Chem. Computer Physics Communications, 2000, 128, 170-177.	7.5	23
104	Variable Scan Rate Cyclic Voltammetry and Theoretical Studies on Tocopherol (Vitamin E) Model Compounds. Journal of Physical Chemistry B, 2008, 112, 6847-6855.	2.6	22
105	Intracule functional models : Part III. The dot intracule and its Fourier transform. Physical Chemistry Chemical Physics, 2008, 10, 3447.	2.8	22
106	Intracule functional models. IV. Basis set effects. Journal of Chemical Physics, 2009, 130, 164110.	3.0	22
107	Correlation energy of the spin-polarized uniform electron gas at high density. Physical Review B, 2011, 84, .	3.2	22
108	Computation of molecular Hartreeâ€“Fock Wigner intracules. Journal of Chemical Physics, 2003, 118, 2033-2038.	3.0	21

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109	Intracule functional models: I. Angle-corrected correlation kernels. Physical Chemistry Chemical Physics, 2007, 9, 5340.	2.8	21
110	Uniform electron gases. II. The generalized local density approximation in one dimension. Journal of Chemical Physics, 2014, 140, 18A524.	3.0	21
111	How well can RMP4 theory treat homolytic fragmentations?. Chemical Physics Letters, 1988, 148, 541-549.	2.6	20
112	Computation and analysis of molecular Hartreeâ€"Fock momentum intracules. Molecular Physics, 2002, 100, 1763-1770.	1.7	20
113	Intracule functional models. V. Recurrence relations for two-electron integrals in position and momentum space. Physical Chemistry Chemical Physics, 2011, 13, 2972-2978.	2.8	20
114	Gaussian Expansions of Orbitals. Journal of Chemical Theory and Computation, 2012, 8, 4891-4898.	5.3	20
115	Atomic and molecular intracules for excited states. Journal of Chemical Physics, 2004, 120, 7290-7297.	3.0	19
116	Long-Lived Radical Cations as Model Compounds for the Reactive One-Electron Oxidation Product of Vitamin E. Journal of Physical Chemistry B, 2008, 112, 10367-10374.	2.6	19
117	Ground state of two electrons on concentric spheres. Physical Review A, 2010, 81, .	2.5	19
118	Empirical density functional and the adsorption of organic molecules on Si(100). Physical Review B, 2003, 67, .	3.2	18
119	Computation and interpretation of molecular Omega intracules. Journal of Chemical Physics, 2007, 127, 014101.	3.0	18
120	Beckeâ€"Wigner : a simple but powerful density functional. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 4337-4341.	1.7	17
121	Advances in methodologies for linear-scaling density functional calculations. Theoretical and Computational Chemistry, 1996, 4, 441-463.	0.4	17
122	Decay behavior of least-squares coefficients in auxiliary basis expansions. Journal of Chemical Physics, 2005, 123, 061101.	3.0	17
123	Mixed Rampâ€"Gaussian Basis Sets. Journal of Chemical Theory and Computation, 2014, 10, 4369-4376.	5.3	17
124	Highly Oxidized Ruthenium Organometallic Compounds. The Synthesis and One-Electron Electrochemical Oxidation of [Cp*RuIVCl2(S2CR)] (Cp* = Î·5-C5Me5, R = NMe2, NEt2, OiPr). Organometallics, 2006, 25, 6134-6141.	2.3	16
125	Performance of Gradient-Corrected and Hybrid Density Functional Theory: Role of the Underlying Local Density Approximation and the Gradient Correction. Journal of Chemical Theory and Computation, 2012, 8, 4899-4906.	5.3	16
126	An optimal point-charge model for molecular electrostatic potentials. Molecular Physics, 2005, 103, 2789-2793.	1.7	15

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127	Resolutions of the Coulomb operator : Part III. Reduced-rank SchrÃ¶dinger equations. Physical Chemistry Chemical Physics, 2009, 11, 9176.	2.8	15
128	Communication: A new approach to dual-basis second-order MÃ¸llerâ€“Plesset calculations. Journal of Chemical Physics, 2011, 134, 081103.	3.0	15
129	Chemistry in one dimension. Physical Chemistry Chemical Physics, 2015, 17, 3196-3206.	2.8	15
130	Two-Electron Integrals over Gaussian Geminals. Journal of Chemical Theory and Computation, 2016, 12, 4915-4924.	5.3	15
131	Model calculations of isotope effects. 10. Temperature-independent isotope effects in hydrogen transfer. Do they signify a bent transition state?. Journal of the American Chemical Society, 1985, 107, 2971-2972.	13.7	14
132	Extracting atoms from molecular electron densities via integral equations. Journal of Chemical Physics, 2004, 120, 7887-7893.	3.0	14
133	Density functional triple jumping. Physical Chemistry Chemical Physics, 2010, 12, 10759.	2.8	14
134	Intracule functional models. Annual Reports on the Progress of Chemistry Section C, 2011, 107, 229.	4.4	14
135	Exact energy of the spin-polarized two-dimensional electron gas at high density. Physical Review B, 2011, 83, .	3.2	14
136	Application of semiempirical molecular orbital theory to cationic intermediates involved in the solvolysis of 1-halobicyclo[n.1.1]alkanes. Journal of Organic Chemistry, 1988, 53, 4354-4357.	3.2	13
137	An improved criterion for evaluating the efficiency of two-electron integral algorithms. Chemical Physics Letters, 1993, 206, 225-228.	2.6	13
138	Many-Electron Integrals over Gaussian Basis Functions. I. Recurrence Relations for Three-Electron Integrals. Journal of Chemical Theory and Computation, 2016, 12, 1735-1740.	5.3	13
139	Rydberg states of the helium atom. International Journal of Quantum Chemistry, 2009, 109, 1915-1919.	2.0	12
140	Hartreeâ€“Fock perturbative corrections for total and reaction energies. Journal of Chemical Physics, 2010, 133, 044116.	3.0	11
141	Resolutions of the Coulomb operator. VI. Computation of auxiliary integrals. Journal of Chemical Physics, 2012, 136, 104102.	3.0	11
142	Coulomb energies via Stewart densities. Chemical Physics Letters, 1998, 286, 226-232.	2.6	10
143	Wigner intracule for the Kellner helium-like ions. International Journal of Quantum Chemistry, 2004, 100, 166-171.	2.0	10
144	Resolutions of the Coulomb Operator: V. The Long-Range Ewald Operator. Journal of Chemical Theory and Computation, 2011, 7, 2353-2357.	5.3	10

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145	Resolutions of the Coulomb Operator: IV. The Spherical Bessel Quasi-Resolution. Journal of Chemical Theory and Computation, 2011, 7, 830-833.	5.3	10
146	Communication: Efficient counterpoise corrections by a perturbative approach. Journal of Chemical Physics, 2011, 135, 081105.	3.0	10
147	Uniform electron gases. III. Low-density gases on three-dimensional spheres. Journal of Chemical Physics, 2015, 143, 084114.	3.0	10
148	Efficient Method for Calculating Effective Core Potential Integrals. Journal of Physical Chemistry A, 2018, 122, 3066-3075.	2.5	10
149	Simple models for describing the fragmentation behavior of multiply charged cations. International Journal of Quantum Chemistry, 1988, 34, 567-573.	2.0	9
150	Comment on â€œa generalized fast multipole approach for Hartree-Fock and density functional computationsâ€• Chemical Physics Letters, 1996, 248, 482-483.	2.6	9
151	Rapid evaluation of two-center two-electron integrals. Journal of Computational Chemistry, 2000, 21, 1505-1510.	3.3	9
152	Finite jellium models. I. Restricted Hartreeâ€“Fock calculations. Journal of Chemical Physics, 2005, 122, 154108.	3.0	9
153	Explicit-r12 correlation methods and local correlation methods. Physical Chemistry Chemical Physics, 2008, 10, 3318.	2.8	9
154	The distribution ofrÂ·pin quantum mechanical systems. New Journal of Physics, 2009, 11, 083015.	2.9	9
155	A remarkable identity involving Bessel functions. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2012, 468, 2667-2681.	2.1	9
156	Q-MP2-OS: MÃllerâ€“Plesset Correlation Energy by Quadrature. Journal of Chemical Theory and Computation, 2020, 16, 1568-1577.	5.3	9
157	Density Functional Partitions. The Journal of Physical Chemistry, 1996, 100, 6348-6353.	2.9	8
158	BFW:Â A Density Functional for Transition Metal Clusters. Journal of Physical Chemistry A, 2007, 111, 2625-2628.	2.5	8
159	Posmom: The Unobserved Observable. Journal of Physical Chemistry Letters, 2010, 1, 1254-1258.	4.6	8
160	Correlation energy of anisotropic quantum dots. Physical Review A, 2011, 84, .	2.5	8
161	Distributions of r₁Â·r₂ and p₁Â·p₂ in Atoms. Journal of Chemical Theory and Computation, 2012, 8, 1657-1662.	5.3	8
162	Leadingâ€•order behavior of the correlation energy in the uniform electron gas. International Journal of Quantum Chemistry, 2012, 112, 1712-1716.	2.0	8

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163	Molecular electronic structure in one-dimensional Coulomb systems. Physical Chemistry Chemical Physics, 2017, 19, 3987-3998.	2.8	8
164	Harmonically trapped jellium. Molecular Physics, 2012, 110, 2337-2342.	1.7	7
165	Communication: Three-electron coalescence points in two and three dimensions. Journal of Chemical Physics, 2015, 143, 181101.	3.0	7
166	MP2[V] â€“ A Simple Approximation to Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2015, 11, 1639-1644.	5.3	7
167	Effects of Coulomb attenuation on chemical properties. Computational and Theoretical Chemistry, 1997, 398-399, 45-54.	1.5	6
168	Methods for constructing Stewart atoms. Computational and Theoretical Chemistry, 2000, 500, 363-374.	1.5	6
169	A point-charge model for electrostatic potentials based on a local projection of multipole moments. Molecular Simulation, 2006, 32, 1249-1253.	2.0	6
170	Resolutions of the Coulomb Operator: VII.ÂEvaluationÂofÂLong-RangeÂCoulombÂandÂExchangeÂMatrices. Journal of Chemical Theory and Computation, 2013, 9, 863-867.	5.3	6
171	Distribution of r12Â· p12in quantum systems. Molecular Physics, 2013, 111, 2414-2426.	1.7	6
172	Basis functions for electronic structure calculations on spheres. Journal of Chemical Physics, 2014, 141, 244102.	3.0	6
173	Chem1D: a software package for electronic structure calculations on one-dimensional systems. Molecular Physics, 2015, 113, 1843-1857.	1.7	6
174	Decomposition of exchange-correlation energies. Chemical Physics Letters, 1999, 312, 511-521.	2.6	4
175	Picosecond time-resolved infrared study of 2-aminopurine ionisation in solution. Photochemical and Photobiological Sciences, 2007, 6, 949.	2.9	4
176	Exact wave functions for concentric two-electron systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 329-333.	2.1	4
177	A generalized Poisson equation and short-range self-interaction energies. Journal of Chemical Physics, 2008, 128, 241101.	3.0	3
178	An Examination of the Relationship Between Transition State Geometry in Hydron Transfer Reactions and the Temperature Dependence of the Primary Kinetic Isotope Effect. Israel Journal of Chemistry, 1985, 26, 378-386.	2.3	2
179	Remembrance: John A. Pople (1925â€“2004). Journal of Chemical Physics, 2004, 120, 9445-9445.	3.0	2
180	Distribution ofrÂ·pin Atomic Systems. Journal of Physical Chemistry A, 2010, 114, 11984-11991.	2.5	2

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181	Diagnostics of molecular orbital quality. Canadian Journal of Chemistry, 2010, 88, 754-758.	1.1	2
182	Intracule Functional Theory. , 2011, , 1-23.		2
183	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
184	Rapid evaluation of twoâ€¢center twoâ€¢electron integrals. Journal of Computational Chemistry, 2000, 21, 1505-1510.	3.3	1
185	Fragmentation Mechanisms for Multiply-Charged Cations. , 1988, , 219-225.		1
186	Reply to Comment on â€œComputing molecular electrostatic potentials with the PRISM algorithmâ€• Chemical Physics Letters, 1994, 218, 595-596.	2.6	0
187	Self-Consistent Hartree-Fock-Wigner Calculations: A Two-Electron-Density Functional Theory. ACS Symposium Series, 2007, , 27-35.	0.5	0
188	Tribute to Leo Radom. Journal of Physical Chemistry A, 2019, 123, 10347-10347.	2.5	0
189	Uniform electron gases. , 2012, , 121-129.		0