Gustavo E Scuseria

List of Publications by Year
in descending order

393	62,669	4146	816
papers	citations	87 h-index	246 g-index

400	400	400	33901
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hybrid functionals based on a screened Coulomb potential. Journal of Chemical Physics, 2003, 118, 8207-8215.	3.0	14,063
2	Climbing the Density Functional Ladder: Nonempirical Metaâ€“Generalized Gradient Approximation Designed for Molecules and Solids. Physical Review Letters, 2003, 91, 146401.	7.8	5,673
3	Assessment of the Perdewâ€“Burkeâ€“Ernzerhof exchange-correlation functional. Journal of Chemical Physics, 1999, 110, 5029-5036.	3.0	3,841
4	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2003, 119, 12129-12137.	3.0	2,157
5	Efficient hybrid density functional calculations in solids: Assessment of the Heydâ€“Scuseriaâ€“Ernzerhof screened Coulomb hybrid functional. Journal of Chemical Physics, 2004, 121, 1187-1192.	3.0	1,932
6	Energy band gaps and lattice parameters evaluated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. Journal of Chemical Physics, 2005, 123, 174101.	3.0	1,604
7	Assessment of a long-range corrected hybrid functional. Journal of Chemical Physics, 2006, 125, 234109.	3.0	1,526
8	An efficient reformulation of the closedâ€shell coupled cluster single and double excitation (CCSD) equations. Journal of Chemical Physics, 1988, 89, 7382-7387.	3.0	1,519
9	Is coupled cluster singles and doubles (CCSD) more computationally intensive than quadratic configuration interaction (QCISD)?. Journal of Chemical Physics, 1989, 90, 3700-3703.	3.0	1,065
10	Importance of short-range versus long-range Hartree-Fock exchange for the performance of hybrid density functionals. Journal of Chemical Physics, 2006, 125, 074106.	3.0	823
11	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. Journal of Chemical Physics, 2005, 123, 062201.	3.0	769
12	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes:â€‰ Conventional versus Long-Range Hybrids. Journal of Chemical Theory and Computation, 2008, 4, 123-135.	5.3	766
13	A novel form for the exchange-correlation energy functional. Journal of Chemical Physics, 1998, 109, 400-410.	3.0	724
14	Assessment and validation of a screened Coulomb hybrid density functional. Journal of Chemical Physics, 2004, 120, 7274-7280.	3.0	698
15	Tests of functionals for systems with fractional electron number. Journal of Chemical Physics, 2007, 126, 154109.	3.0	559
16	The indirect to direct band gap transition in multilayered MoS2 as predicted by screened hybrid density functional theory. Applied Physics Letters, 2011, 99, .	3.3	519
17	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. Journal of Chemical Physics, 2004, 120, 6898-6911.	3.0	431
18	Can short-range hybrids describe long-range-dependent properties?. Journal of Chemical Physics, 2009, 131, 044108.	3.0	426

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19	Understanding band gaps of solids in generalized Kohnâ€“Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
20	Linear Scaling Density Functional Calculations with Gaussian Orbitals. Journal of Physical Chemistry A, 1999, 103, 4782-4790.	2.5	422
21	Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms. Physical Review X, 2015, 5, .	8.9	398
22	Linear scaling second-order Mollerâ€“Plesset theory in the atomic orbital basis for large molecular systems. Journal of Chemical Physics, 1999, 110, 3660-3671.	3.0	389
23	Screened hybrid density functionals for solid-state chemistry and physics. Physical Chemistry Chemical Physics, 2009, 11, 443-454.	2.8	384
24	Spurious fractional charge on dissociated atoms: Pervasive and resilient self-interaction error of common density functionals. Journal of Chemical Physics, 2006, 125, 194112.	3.0	383
25	Analytic evaluation of energy gradients for the single and double excitation coupled cluster (CCSD) wave function: Theory and application. Journal of Chemical Physics, 1987, 87, 5361-5373.	3.0	378
26	Predicting Band Gaps with Hybrid Density Functionals. Journal of Physical Chemistry Letters, 2016, 7, 4165-4170.	4.6	369
27	The closedâ€shell coupled cluster single and double excitation (CCSD) model for the description of electron correlation. A comparison with configuration interaction (CISD) results. Journal of Chemical Physics, 1987, 86, 2881-2890.	3.0	316
28	Linear scaling coupled cluster and perturbation theories in the atomic orbital basis. Journal of Chemical Physics, 1999, 111, 8330-8343.	3.0	313
29	Local hybrid functionals. Journal of Chemical Physics, 2003, 118, 1068-1073.	3.0	298
30	Half-metallic graphene nanodots: A comprehensive first-principles theoretical study. Physical Review B, 2008, 77, .	3.2	290
31	Density functionals that are one- and two- are not always many-electron self-interaction-free, as shown for H2+, He2+, LiH+, and Ne2+. Journal of Chemical Physics, 2007, 126, 104102.	3.0	274
32	Covalency in the actinide dioxides: Systematic study of the electronic properties using screened hybrid density functional theory. Physical Review B, 2007, 76, .	3.2	266
33	The ground state correlation energy of the random phase approximation from a ring coupled cluster doubles approach. Journal of Chemical Physics, 2008, 129, 231101.	3.0	261
34	Accurate treatment of solids with the HSE screened hybrid. Physica Status Solidi (B): Basic Research, 2011, 248, 767-774.	1.5	258
35	Analytic evaluation of energy gradients for the singles and doubles coupled cluster method including perturbative triple excitations: Theory and applications to FOOF and Cr2. Journal of Chemical Physics, 1991, 94, 442-447.	3.0	253
36	Linear scaling conjugate gradient density matrix search as an alternative to diagonalization for first principles electronic structure calculations. Journal of Chemical Physics, 1997, 106, 5569-5577.	3.0	247

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37	Generalized gradient approximation model exchange holes for range-separated hybrids. Journal of Chemical Physics, 2008, 128, 194105.	3.0	238
38	Coupled cluster energy derivatives. Analytic Hessian for the closedâ€shell coupled cluster singles and doubles wave function: Theory and applications. Journal of Chemical Physics, 1990, 92, 4924-4940.	3.0	222
39	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. Physical Review A, 2008, 78, .	2.5	221
40	Atomic orbital Laplace-transformed second-order MÃ¸llerâ€“Plesset theory for periodic systems. Journal of Chemical Physics, 2001, 115, 9698-9707.	3.0	193
41	Projected Hartreeâ€“Fock theory. Journal of Chemical Physics, 2012, 136, 164109.	3.0	191
42	Density Functional Theory Studies of the Electronic Structure of Solid State Actinide Oxides. Chemical Reviews, 2013, 113, 1063-1096.	47.7	191
43	Role of sp3 carbon and 7-membered rings in fullerene annealing and fragmentation. Nature, 1993, 366, 665-667.	27.8	188
44	Comparison of coupledâ€cluster results with a hybrid of Hartreeâ€“Fock and density functional theory. Journal of Chemical Physics, 1992, 97, 7528-7530.	3.0	181
45	Towards the Solution of the Many-Electron Problem in Real Materials: Equation of State of the Hydrogen Chain with State-of-the-Art Many-Body Methods. Physical Review X, 2017, 7, .	8.9	171
46	Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. Physical Review Letters, 2013, 111, 106401.	7.8	168
47	Ab initio theoretical predictions of C28, C28H4, C28F4, (Ti@C28)H4, and M@C28 (M=Mg, Al, Si, S, Ca, Sc,) Tj ETQq1 1 0.784314 rgB	3.0	158
48	Long-range-corrected hybrids including random phase approximation correlation. Journal of Chemical Physics, 2009, 130, 081105.	3.0	158
49	Assessment of a Middle-Range Hybrid Functional. Journal of Chemical Theory and Computation, 2008, 4, 1254-1262.	5.3	155
50	The vibrational frequencies of ozone. Journal of Chemical Physics, 1990, 93, 489-494.	3.0	152
51	The importance of middle-range Hartree-Fock-type exchange for hybrid density functionals. Journal of Chemical Physics, 2007, 127, 221103.	3.0	152
52	Edge effects in finite elongated graphene nanoribbons. Physical Review B, 2007, 76, .	3.2	148
53	Projected quasiparticle theory for molecular electronic structure. Journal of Chemical Physics, 2011, 135, 124108.	3.0	148
54	Accurate solid-state band gaps via screened hybrid electronic structure calculations. Journal of Chemical Physics, 2008, 129, 011102.	3.0	147

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55	Seniority zero pair coupled cluster doubles theory. Journal of Chemical Physics, 2014, 140, 214113.	3.0	147
56	The optimization of molecular orbitals for coupled cluster wavefunctions. Chemical Physics Letters, 1987, 142, 354-358.	2.6	144
57	Accelerating the convergence of the coupled-cluster approach. Chemical Physics Letters, 1986, 130, 236-239.	2.6	143
58	Exchange and correlation in open systems of fluctuating electron number. Physical Review A, 2007, 76, .	2.5	140
59	A quantitative study of the scaling properties of the Hartreeâ€“Fock method. Journal of Chemical Physics, 1995, 102, 8448-8452.	3.0	139
60	Semiempirical methods with conjugate gradient density matrix search to replace diagonalization for molecular systems containing thousands of atoms. Journal of Chemical Physics, 1997, 107, 425-431.	3.0	138
61	Assessment of correlation energies based on the random-phase approximation. New Journal of Physics, 2012, 14, 043002.	2.9	137
62	Hybrid functionals with local range separation. Journal of Chemical Physics, 2008, 129, 124103.	3.0	134
63	Mechanically induced defects and strength of BN nanotubes. Physical Review B, 2002, 65, .	3.2	132
64	Comparison of screened hybrid density functional theory to diffusion Monte Carlo in calculations of total energies of silicon phases and defects. Physical Review B, 2006, 74, .	3.2	131
65	Hybrid functionals including random phase approximation correlation and second-order screened exchange. Journal of Chemical Physics, 2010, 132, 094103.	3.0	131
66	Exact parameterization of fermionic wave functions via unitary coupled cluster theory. Journal of Chemical Physics, 2019, 151, 244112.	3.0	124
67	Seniority and orbital symmetry as tools for establishing a full configuration interaction hierarchy. Journal of Chemical Physics, 2011, 135, 044119.	3.0	121
68	What is the best alternative to diagonalization of the Hamiltonian in large scale semiempirical calculations?. Journal of Chemical Physics, 1999, 110, 1321-1328.	3.0	120
69	Assessment of long-range corrected functionals performance for nâ†'Ï€* transitions in organic dyes. Journal of Chemical Physics, 2007, 127, 094102.	3.0	119
70	Structure and Conformational Behavior of Biopolymers by Density Functional Calculations Employing Periodic Boundary Conditions. I. The Case of Polyglycine, Polyalanine, and Poly-Î±-aminoisobutyric Acid in Vacuo. Journal of the American Chemical Society, 2001, 123, 3311-3322.	13.7	117
71	The meta-GGA functional: Thermochemistry with a kinetic energy density dependent exchange-correlation functional. Journal of Chemical Physics, 2000, 112, 2643-2649.	3.0	114
72	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. Physical Review B, 2013, 88, .	3.2	113

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73	Multideterminant Wave Functions in Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2012, 8, 2181-2188.	5.3	110
74	Seniority-based coupled cluster theory. Journal of Chemical Physics, 2014, 141, 244104.	3.0	110
75	The photodissociation of formaldehyde: A coupled cluster study including connected triple excitations of the transition state barrier height for H2COâ†'H2+CO. Journal of Chemical Physics, 1989, 90, 3629-3636.	3.0	108
76	Progress in the development of exchange-correlation functionals. , 2005, , 669-724.		108
77	Doping of Polyaniline by Acidâ^'Base Chemistry:Â Density Functional Calculations with Periodic Boundary Conditions. Journal of the American Chemical Society, 2005, 127, 11318-11327.	13.7	107
78	Improving self-consistent field convergence by varying occupation numbers. Journal of Chemical Physics, 1999, 110, 695-700.	3.0	106
79	A systematic theoretical study of harmonic vibrational frequencies: The single and double excitation coupled cluster (CCSD) method. Journal of Chemical Physics, 1988, 89, 360-366.	3.0	105
80	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. Physical Review A, 2008, 77, .	2.5	104
81	Density matrix embedding from broken symmetry lattice mean fields. Physical Review B, 2014, 89, .	3.2	103
82	Can Single-Reference Coupled Cluster Theory Describe Static Correlation?. Journal of Chemical Theory and Computation, 2015, 11, 3171-3179.	5.3	103
83	Blind test of density-functional-based methods on intermolecular interaction energies. Journal of Chemical Physics, 2016, 145, 124105.	3.0	97
84	Performance of recently developed kinetic energy density functionals for the calculation of hydrogen binding strengths and hydrogen-bonded structures. Theoretical Chemistry Accounts, 2000, 104, 439-444.	1.4	96
85	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. Chemical Physics Letters, 2008, 465, 226-229.	2.6	96
86	Hartreeâ€"Fock orbitals significantly improve the reaction barrier heights predicted by semilocal density functionals. Journal of Chemical Physics, 2008, 128, 244112.	3.0	89
87	Quasiparticle coupled cluster theory for pairing interactions. Physical Review C, 2014, 89, .	2.9	88
88	Testing density functionals for structural phase transitions of solids under pressure: Si, SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>, and Zr. Physical Review B, 2013, 88, .	3.2	87
89	Kinetic energy density dependent approximations to the exchange energy. Journal of Chemical Physics, 1999, 111, 911-915.	3.0	83
90	Noncollinear magnetism in density functional calculations. Physical Review B, 2007, 75, .	3.2	83

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91	Many-electron self-interaction and spin polarization errors in local hybrid density functionals. Journal of Chemical Physics, 2010, 133, 134116.	3.0	83
92	Spinâ€“spin coupling constants of CO and N2. Journal of Chemical Physics, 1987, 87, 2138-2142.	3.0	82
93	Long-range-corrected hybrid density functionals including random phase approximation correlation: Application to noncovalent interactions. Journal of Chemical Physics, 2009, 131, 034110.	3.0	82
94	Strong correlations via constrained-pairing mean-field theory. Journal of Chemical Physics, 2009, 131, 121102.	3.0	82
95	Entanglement and Polyradical Character of Polycyclic Aromatic Hydrocarbons Predicted by Projected Hartreeâ€“Fock Theory. Journal of Physical Chemistry B, 2013, 117, 12750-12758.	2.6	82
96	The connection between self-interaction and static correlation: a random phase approximation perspective. Molecular Physics, 2010, 108, 2511-2517.	1.7	79
97	The elusive signature of CH5+. Nature, 1993, 366, 512-513.	27.8	76
98	Particle-particle and quasiparticle random phase approximations: Connections to coupled cluster theory. Journal of Chemical Physics, 2013, 139, 104113.	3.0	76
99	Electron correlation in solids via density embedding theory. Journal of Chemical Physics, 2014, 141, 054113.	3.0	75
100	Long-Range-Corrected Hybrids Based on a New Model Exchange Hole. Journal of Chemical Theory and Computation, 2009, 5, 754-762.	5.3	72
101	Ab initio molecular dynamics: Propagating the density matrix with gaussian orbitals. IV. Formal analysis of the deviations from born-oppenheimer dynamics. Israel Journal of Chemistry, 2002, 42, 191-202.	2.3	71
102	On the difference between variational and unitary coupled cluster theories. Journal of Chemical Physics, 2018, 148, 044107.	3.0	70
103	Thermodynamics of yield in boron nitride nanotubes. Physical Review B, 2003, 68, .	3.2	68
104	Self-consistent generalized Kohn-Sham local hybrid functionals of screened exchange: Combining local and range-separated hybridization. Journal of Chemical Physics, 2008, 129, 124110.	3.0	68
105	Assessment of Density Functionals for Predicting One-Bond Carbonâ^'Hydrogen NMR Spinâ^'Spin Coupling Constants. Journal of Chemical Theory and Computation, 2005, 1, 541-545.	5.3	66
106	Dispersion in the Mott insulator UO₂: A comparison of photoemission spectroscopy and screened hybrid density functional theory. Journal of Computational Chemistry, 2008, 29, 2288-2294.	3.3	65
107	An assessment for the full coupled cluster method including all single, double, and triple excitations: The diatomic molecules LiH, Li2, BH, LiF, C2, BeO, CN+, BF, NO+, and F2. Journal of Chemical Physics, 1990, 92, 568-573.	3.0	64
108	Generalized Hartreeâ€“Fock Description of Molecular Dissociation. Journal of Chemical Theory and Computation, 2011, 7, 2667-2674.	5.3	64

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109	Assessment of simple exchange-correlation energy functionals of the one-particle density matrix. Journal of Chemical Physics, 2002, 117, 2489-2495.	3.0	62
110	Assessment of long-range corrected functionals for the prediction of non-linear optical properties of organic materials. Chemical Physics Letters, 2013, 575, 122-125.	2.6	62
111	Mott transition of MnO under pressure: A comparison of correlated band theories. Physical Review B, 2006, 74, .	3.2	60
112	Resolution of the identity atomic orbital Laplace transformed second order MÃ¸llerâ€“Plesset theory for nonconducting periodic systems. Physical Chemistry Chemical Physics, 2008, 10, 3421.	2.8	60
113	Optical band gap of NpO2 and PuO2 from optical absorbance of epitaxial films. Journal of Applied Physics, 2013, 113, .	2.5	58
114	Scaling reduction of the perturbative triples correction (T) to coupled cluster theory via Laplace transform formalism. Journal of Chemical Physics, 2000, 113, 10451-10458.	3.0	57
115	Why are buckyonions round?. Theoretical Chemistry Accounts, 1998, 99, 29-33.	1.4	56
116	Projected coupled cluster theory. Journal of Chemical Physics, 2017, 147, 064111.	3.0	56
117	Abinitiotheoretical study of small GaAs clusters. Journal of Chemical Physics, 1991, 95, 6602-6606.	3.0	54
118	Genetic algorithms: A robust scheme for geometry optimizations and global minimum structure problems. Journal of Computational Chemistry, 1995, 16, 729-742.	3.3	54
119	Local hybrid functionals based on density matrix products. Journal of Chemical Physics, 2007, 127, 164117.	3.0	54
120	Can Gap Tuning Schemes of Long-Range Corrected Hybrid Functionals Improve the Description of Hyperpolarizabilities?. Journal of Physical Chemistry B, 2015, 119, 1202-1212.	2.6	54
121	The conformational behavior of polyglycine as predicted by a density functional model with periodic boundary conditions. Journal of Chemical Physics, 2001, 114, 2541-2549.	3.0	53
122	Theoretical study of the electronic properties of narrow single-walled carbon nanotubes: Beyond the local density approximation. Journal of Chemical Physics, 2004, 121, 10376-10379.	3.0	53
123	Effect of oxygen chemisorption on the energy band gap of a chiral semiconducting single-walled carbon nanotube. Chemical Physics Letters, 2004, 389, 289-292.	2.6	53
124	Pair extended coupled cluster doubles. Journal of Chemical Physics, 2015, 142, 214116.	3.0	53
125	Polynomial similarity transformation theory: A smooth interpolation between coupled cluster doubles and projected BCS applied to the reduced BCS Hamiltonian. Physical Review B, 2016, 93, .	3.2	53
126	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. Physical Review A, 2008, 77, .	2.5	52

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127	Can Short- and Middle-Range Hybrids Describe the Hyperpolarizabilities of Long-Range Charge-Transfer Compounds?. Journal of Physical Chemistry A, 2014, 118, 11787-11796.	2.5	52
128	Structural phase transitions of the metal oxide perovskites SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>, LaAlO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>, and LaTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	3.2	51
129	Multi-component symmetry-projected approach for molecular ground state correlations. Journal of Chemical Physics, 2013, 139, 204102.	3.0	51
130	Calculation of spectra and spin-spin coupling constants using a coupled-cluster polarization propagator method. International Journal of Quantum Chemistry, 1987, 32, 475-485.	2.0	50
131	An efficient finite field approach for calculating static electric polarizabilities of periodic systems. Journal of Chemical Physics, 2000, 113, 7779-7785.	3.0	50
132	Evaluation of Range-Separated Hybrid and Other Density Functional Approaches on Test Sets Relevant for Transition Metal-Based Homogeneous Catalysts. Journal of Physical Chemistry A, 2009, 113, 11742-11749.	2.5	50
133	Tensor-structured coupled cluster theory. Journal of Chemical Physics, 2017, 147, 184113.	3.0	48
134	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. Physical Review B, 2009, 80, .	3.2	47
135	The infrared spectrum of cyclotetraoxygen, O4: A theoretical investigation employing the single and double excitation coupled cluster method. Journal of Chemical Physics, 1990, 92, 6077-6080.	3.0	45
136	Description of magnetic interactions in strongly correlated solids via range-separated hybrid functionals. Physical Review B, 2009, 79, .	3.2	44
137	Multireference symmetry-projected variational approaches for ground and excited states of the one-dimensional Hubbard model. Physical Review B, 2013, 87, .	3.2	44
138	Linear scaling density matrix search based onsignmatrices. Journal of Chemical Physics, 2000, 113, 6035-6041.	3.0	43
139	Optimization of density matrix functionals by the Hartreeâ€“Fockâ€“Bogoliubov method. Journal of Chemical Physics, 2002, 117, 11107-11112.	3.0	43
140	Symmetry-projected wave functions in quantum Monte Carlo calculations. Physical Review B, 2014, 89, .	3.2	43
141	Polyradical Character and Spin Frustration in Fullerene Molecules: An Ab Initio Non-Collinear Hartreeâ€“Fock Study. Journal of Physical Chemistry A, 2014, 118, 9925-9940.	2.5	43
142	Nuclear magnetic resonance shielding tensors calculated with kinetic energy density-dependent exchange-correlation functionals. Chemical Physics Letters, 2004, 390, 408-412.	2.6	42
143	Energy storage capacity of polymeric nitrogen. Molecular Physics, 2006, 104, 745-749.	1.7	42
144	Parameterized local hybrid functionals from density-matrix similarity metrics. Journal of Chemical Physics, 2008, 128, 084111.	3.0	42

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145	Symmetry-projected variational approach for ground and excited states of the two-dimensional Hubbard model. Physical Review B, 2012, 85, .	3.2	42
146	Constrained-pairing mean-field theory. II. Exact treatment of dissociations to nondegenerate orbitals. Journal of Chemical Physics, 2009, 131, 164119.	3.0	41
147	Range-separated local hybrids. Journal of Chemical Physics, 2010, 132, 224106.	3.0	41
148	A computational study of the nonlinear optical properties of carbazole derivatives: theory refines experiment. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	41
149	Ordering of the Oâ€“O stretching vibrational frequencies in ozone. Journal of Chemical Physics, 1989, 90, 5635-5637.	3.0	40
150	Range separated hybrids of pair coupled cluster doubles and density functionals. Physical Chemistry Chemical Physics, 2015, 17, 22412-22422.	2.8	40
151	Characterization of Six Isomers of [84]Fullerene C84by Electrochemistry, Electron Spin Resonance Spectroscopy, and Molecular Energy Levels Calculations. Journal of Physical Chemistry A, 2001, 105, 4627-4632.	2.5	38
152	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. Physical Review A, 2007, 76, .	2.5	37
153	Range-Separated Brueckner Coupled Cluster Doubles Theory. Physical Review Letters, 2014, 112, 133002.	7.8	37
154	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. Physical Review B, 2017, 95, .	3.2	37
155	Correlating AGP on a quantum computer. Quantum Science and Technology, 2021, 6, 014004.	5.8	37
156	All-Electron Hybrid Density Functional Calculations on UFn and UCln (n = 1â^'6). Journal of Chemical Theory and Computation, 2005, 1, 612-616.	5.3	36
157	Regularized Gradient Expansion for Atoms, Molecules, and Solids. Journal of Chemical Theory and Computation, 2009, 5, 763-769.	5.3	36
158	Modeling of the cubic and antiferrodistortive phases of SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>with screened hybrid density functional theory. Physical Review B, 2011, 84, .	3.2	36
159	Coupled cluster channels in the homogeneous electron gas. Journal of Chemical Physics, 2014, 140, 124102.	3.0	36
160	Seniority number description of potential energy surfaces: Symmetric dissociation of water, N2, C2, and Be2. Journal of Chemical Physics, 2015, 143, 094105.	3.0	36
161	Synergy between pair coupled cluster doubles and pair density functional theory. Journal of Chemical Physics, 2015, 142, 044109.	3.0	36
162	Comparison of conjugate gradient density matrix search and Chebyshev expansion methods for avoiding diagonalization in large-scale electronic structure calculations. Journal of Chemical Physics, 1998, 109, 3308-3312.	3.0	35

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163	A coupled cluster study of the classical barrier height of the F+H2â†'FH+H reaction. Journal of Chemical Physics, 1991, 95, 7426-7436.	3.0	33
164	A comparison of the coupled cluster and internallyâ€contracted averaged coupledâ€pairâ€functional levels of theory for the calculation of the MCH2+ binding energies for M=Sc to Cu. Journal of Chemical Physics, 1992, 97, 7471-7473.	3.0	33
165	Local hybrids as a perturbation to global hybrid functionals. Journal of Chemical Physics, 2009, 131, 154112.	3.0	33
166	Long-range-corrected hybrids using a range-separated Perdew-Burke-Ernzerhof functional and random phase approximation correlation. Journal of Chemical Physics, 2011, 135, 094105.	3.0	33
167	Exploring Copper Oxide Cores Using the Projected Hartreeâ€"Fock Method. Journal of Chemical Theory and Computation, 2012, 8, 4944-4949.	5.3	33
168	Capturing static and dynamic correlations by a combination of projected Hartree-Fock and density functional theories. Journal of Chemical Physics, 2013, 138, 134102.	3.0	31
169	Sign problem in full configuration interaction quantum Monte Carlo: Linear and sublinear representation regimes for the exact wave function. Physical Review B, 2014, 90, .	3.2	31
170	Geminal-based configuration interaction. Journal of Chemical Physics, 2019, 151, .	3.0	31
171	Constrained-pairing mean-field theory. III. Inclusion of density functional exchange and correlation effects via alternative densities. Journal of Chemical Physics, 2010, 132, 024111.	3.0	30
172	Merging symmetry projection methods with coupled cluster theory: Lessons from the Lipkin model Hamiltonian. Journal of Chemical Physics, 2017, 146, 054110.	3.0	30
173	Thermofield Theory for Finite-Temperature Coupled Cluster. Journal of Chemical Theory and Computation, 2019, 15, 6127-6136.	5.3	30
174	Thermofield theory for finite-temperature quantum chemistry. Journal of Chemical Physics, 2019, 150, 154109.	3.0	30
175	Range definitions for Gaussian-type charge distributions in fast multipole methods. Journal of Chemical Physics, 1999, 111, 2351-2356.	3.0	29
176	The role of the reference state in long-range random phase approximation correlation. Journal of Chemical Physics, 2009, 131, 154106.	3.0	29
177	Coulomb-only second-order perturbation theory in long-range-corrected hybrid density functionals. Physical Chemistry Chemical Physics, 2009, 11, 9677.	2.8	29
178	Photochromic and nonlinear optical properties of fulgides: A density functional theory study. Computational and Theoretical Chemistry, 2013, 1022, 82-85.	2.5	29
179	Predicting Singletâ€"Triplet Energy Splittings with Projected Hartreeâ€"Fock Methods. Journal of Physical Chemistry A, 2013, 117, 8073-8080.	2.5	29
180	Ring-locking enables selective anhydrosugar synthesis from carbohydrate pyrolysis. Green Chemistry, 2016, 18, 5438-5447.	9.0	29

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