Gustavo E Scuseria

List of Publications by Year in Descending Order

274 papers	51,882 citations	83 h-index	226 g-index
400 ext. papers	57,321 ext. citations	5.4 avg, IF	7.93 L-index

#	Paper	IF	Citations
274	Thermal coupled cluster theory for SU(2) systems. *Physical Review B*, **2022**, 105,	3.3	3
273	A power series approximation in symmetry projected coupled cluster theory.. *Journal of Chemical Physics*, **2022**, 156, 104105	3.9	0
272	Correlating AGP on a quantum computer. *Quantum Science and Technology*, **2021**, 6, 014004	5.5	11
271	Construction of linearly independent non-orthogonal AGP states. *Journal of Chemical Physics*, **2021**, 154, 114112	3.9	7
270	Exploring non-linear correlators on AGP. *Journal of Chemical Physics*, **2021**, 154, 074113	3.9	11
269	Advancing solid-state band gap predictions. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	1
268	Correlating the antisymmetrized geminal power wave function. *Journal of Chemical Physics*, **2020**, 153, 084111	3.9	16
267	Confronting Racism in Chemistry Journals. *ACS Applied Nano Materials*, **2020**, 3, 6131-6133	5.6	
266	Confronting Racism in Chemistry Journals. *ACS Applied Polymer Materials*, **2020**, 2, 2496-2498	4.3	
265	Confronting Racism in Chemistry Journals. *Organometallics*, **2020**, 39, 2331-2333	3.8	
264	Update to Our Reader, Reviewer, and Author Communities April 2020. *Energy & Fuels*, **2020**, 34, 5107-5108	4.1	
263	Update to Our Reader, Reviewer, and Author Communities April 2020. *Organometallics*, **2020**, 39, 1665-1666	3.8	
262	Confronting Racism in Chemistry Journals. *Journal of Chemical Health and Safety*, **2020**, 27, 198-200	1.7	
261	Wave function methods for canonical ensemble thermal averages in correlated many-fermion systems. *Journal of Chemical Physics*, **2020**, 153, 124115	3.9	9
260	Geminal Replacement Models Based on AGP. *Journal of Chemical Theory and Computation*, **2020**, 16, 6358-6367	5.4	10
259	Assessing combinations of singlet-paired coupled cluster and density functional theory for treating electron correlation in closed and open shells. *Molecular Physics*, **2020**, 118, 1615144	1.7	1
258	Geminal-based configuration interaction. *Journal of Chemical Physics*, **2019**, 151, 051101	3.9	20

257	Thermofield Theory for Finite-Temperature Coupled Cluster. *Journal of Chemical Theory and Computation*, **2019**, 15, 6127-6136	6.4	24
256	Thermofield theory for finite-temperature quantum chemistry. *Journal of Chemical Physics*, **2019**, 150, 154109	3.9	23
255	Polynomial-product states: A symmetry-projection-based factorization of the full coupled cluster wavefunction in terms of polynomials of double excitations. *Journal of Chemical Physics*, **2019**, 150, 144108	3.9	6
254	Efficient evaluation of AGP reduced density matrices. *Journal of Chemical Physics*, **2019**, 151, 184103	3.9	18
253	Exact parameterization of fermionic wave functions via unitary coupled cluster theory. *Journal of Chemical Physics*, **2019**, 151, 244112	3.9	63
252	On the difference between variational and unitary coupled cluster theories. *Journal of Chemical Physics*, **2018**, 148, 044107	3.9	41
251	Hartree-Fock symmetry breaking around conical intersections. *Journal of Chemical Physics*, **2018**, 148, 024109	3.9	8
250	Influence of broken-pair excitations on the exact pair wavefunction. *Molecular Physics*, **2018**, 116, 186-193	1.7	7
249	Magnetic Structure of Density Matrices. *Journal of Chemical Theory and Computation*, **2018**, 14, 649-659	6.4	9
248	Projected coupled cluster theory: Optimization of cluster amplitudes in the presence of symmetry projection. *Journal of Chemical Physics*, **2018**, 149, 164108	3.9	16
247	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. *Physical Review B*, **2017**, 95,	3.3	32
246	Merging symmetry projection methods with coupled cluster theory: Lessons from the Lipkin model Hamiltonian. *Journal of Chemical Physics*, **2017**, 146, 054110	3.9	24
245	Understanding band gaps of solids in generalized Kohn-Sham theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2801-2806	11.5	280
244	Projected Hartree-Fock theory as a polynomial of particle-hole excitations and its combination with variational coupled cluster theory. *Journal of Chemical Physics*, **2017**, 146, 184105	3.9	19
243	Semilocal exchange hole with an application to range-separated density functionals. *Physical Review B*, **2017**, 95,	3.3	18
242	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,	9.1	121
241	Spin-projected generalized Hartree-Fock method as a polynomial of particle-hole excitations. *Physical Review A*, **2017**, 96,	2.6	9
240	Combining symmetry collective states with coupled-cluster theory: Lessons from the Agassi model Hamiltonian. *Physical Review C*, **2017**, 95,	2.7	11

239	Projected coupled cluster theory. *Journal of Chemical Physics*, **2017**, 147, 064111	3.9	43
238	Electronic Structure and Properties of Berkelium Iodates. *Journal of the American Chemical Society*, **2017**, 139, 13361-13375	16.4	18
237	Attenuated coupled cluster: a heuristic polynomial similarity transformation incorporating spin symmetry projection into traditional coupled cluster theory. *Molecular Physics*, **2017**, 115, 2673-2683	1.7	9
236	Spin polynomial similarity transformation for repulsive Hamiltonians: interpolating between coupled cluster and spin-projected unrestricted Hartree-Fock. *Physical Chemistry Chemical Physics*, **2017**, 19, 22385-22394	3.6	2
235	Tensor-structured coupled cluster theory. *Journal of Chemical Physics*, **2017**, 147, 184113	3.9	31
234	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,	3.3	41
233	Ring-locking enables selective anhydrosugar synthesis from carbohydrate pyrolysis. *Green Chemistry*, **2016**, 18, 5438-5447	10	24
232	Communication: Projected Hartree Fock theory as a polynomial similarity transformation theory of single excitations. *Journal of Chemical Physics*, **2016**, 145, 111102	3.9	27
231	The two pillars: density and spin-density functional theories. *Molecular Physics*, **2016**, 114, 928-931	1.7	6
230	Graphene Nanoribbons-Based Ultrasensitive Chemical Detectors. *Journal of Physical Chemistry C*, **2016**, 120, 3791-3797	3.8	10
229	Combinations of coupled cluster, density functionals, and the random phase approximation for describing static and dynamic correlation, and van der Waals interactions. *Molecular Physics*, **2016**, 114, 997-1018	1.7	22
228	Recoupling the singlet- and triplet-pairing channels in single-reference coupled cluster theory. *Journal of Chemical Physics*, **2016**, 145, 134103	3.9	9
227	Blind test of density-functional-based methods on intermolecular interaction energies. *Journal of Chemical Physics*, **2016**, 145, 124105	3.9	76
226	Singlet-paired coupled cluster theory for open shells. *Journal of Chemical Physics*, **2016**, 144, 244117	3.9	16
225	Using full configuration interaction quantum Monte Carlo in a seniority zero space to investigate the correlation energy equivalence of pair coupled cluster doubles and doubly occupied configuration interaction. *Journal of Chemical Physics*, **2016**, 144, 094112	3.9	21
224	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. *Journal of Chemical Physics*, **2016**, 145, 234306	3.9	23
223	Predicting Band Gaps with Hybrid Density Functionals. *Journal of Physical Chemistry Letters*, **2016**, 7, 4165-4170	6.4	286
222	Range separated hybrids of pair coupled cluster doubles and density functionals. *Physical Chemistry Chemical Physics*, **2015**, 17, 22412-22	3.6	34

221	Can Single-Reference Coupled Cluster Theory Describe Static Correlation?. *Journal of Chemical Theory and Computation*, **2015**, 11, 3171-9	6.4	77
220	Synergy between pair coupled cluster doubles and pair density functional theory. *Journal of Chemical Physics*, **2015**, 142, 044109	3.9	31
219	On the equivalence of LIST and DIIS methods for convergence acceleration. *Journal of Chemical Physics*, **2015**, 142, 164104	3.9	6
218	Pair extended coupled cluster doubles. *Journal of Chemical Physics*, **2015**, 142, 214116	3.9	43
217	Can gap tuning schemes of long-range corrected hybrid functionals improve the description of hyperpolarizabilities?. *Journal of Physical Chemistry B*, **2015**, 119, 1202-12	3.4	47
216	Lie algebraic similarity transformed Hamiltonians for lattice model systems. *Physical Review B*, **2015**, 91,	3.3	11
215	Cluster-based mean-field and perturbative description of strongly correlated fermion systems: Application to the one- and two-dimensional Hubbard model. *Physical Review B*, **2015**, 92,	3.3	10
214	Actinide chemistry using singlet-paired coupled cluster and its combinations with density functionals. *Journal of Chemical Physics*, **2015**, 143, 244106	3.9	15
213	Seniority number description of potential energy surfaces: Symmetric dissociation of water, N2, C2, and Be2. *Journal of Chemical Physics*, **2015**, 143, 094105	3.9	32
212	Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms. *Physical Review X*, **2015**, 5,	9.1	269
211	A computational study of the nonlinear optical properties of carbazole derivatives: theory refines experiment. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	30
210	Electron correlation in solids via density embedding theory. *Journal of Chemical Physics*, **2014**, 141, 054113	3.9	66
209	Potential energy curves for Mo2: multi-component symmetry-projected Hartree–Fock and beyond. *Molecular Physics*, **2014**, 112, 1938-1946	1.7	8
208	Electronic correlation without double counting via a combination of spin projected Hartree-Fock and density functional theories. *Journal of Chemical Physics*, **2014**, 140, 244102	3.9	23
207	Polyradical character and spin frustration in fullerene molecules: an ab initio non-collinear Hartree-Fock study. *Journal of Physical Chemistry A*, **2014**, 118, 9925-40	2.8	36
206	Prediction of the linear and nonlinear optical properties of tetrahydronaphthalone derivatives via long-range corrected hybrid functionals. *Molecular Physics*, **2014**, 112, 3165-3172	1.7	19
205	Quasiparticle coupled cluster theory for pairing interactions. *Physical Review C*, **2014**, 89,	2.7	76
204	Seniority-based coupled cluster theory. *Journal of Chemical Physics*, **2014**, 141, 244104	3.9	86

203	Analytic energy gradient for the projected Hartree-Fock method. *Journal of Chemical Physics*, **2014**, 140, 204101	3.9	15
202	Symmetry-projected wave functions in quantum Monte Carlo calculations. *Physical Review B*, **2014**, 89,	3.3	36
201	Seniority zero pair coupled cluster doubles theory. *Journal of Chemical Physics*, **2014**, 140, 214113	3.9	119
200	Sign problem in full configuration interaction quantum Monte Carlo: Linear and sublinear representation regimes for the exact wave function. *Physical Review B*, **2014**, 90,	3.3	28
199	Variational description of the ground state of the repulsive two-dimensional Hubbard model in terms of nonorthogonal symmetry-projected Slater determinants. *Physical Review B*, **2014**, 90,	3.3	9
198	Range-separated Brueckner coupled cluster doubles theory. *Physical Review Letters*, **2014**, 112, 133002	7.4	30
197	Can short- and middle-range hybrids describe the hyperpolarizabilities of long-range charge-transfer compounds?. *Journal of Physical Chemistry A*, **2014**, 118, 11787-96	2.8	45
196	Density matrix embedding from broken symmetry lattice mean fields. *Physical Review B*, **2014**, 89,	3.3	90
195	Coupled cluster channels in the homogeneous electron gas. *Journal of Chemical Physics*, **2014**, 140, 124102	3.9	31
194	Multireference symmetry-projected variational approximation for the ground state of the doped one-dimensional Hubbard model. *Physical Review B*, **2014**, 89,	3.3	5
193	Nonlinear optical properties of DPO and DMPO: a theoretical and computational study. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	21
192	Density functionals that recognize covalent, metallic, and weak bonds. *Physical Review Letters*, **2013**, 111, 106401	7.4	143
191	Photochromic and nonlinear optical properties of fulgides: A density functional theory study. *Computational and Theoretical Chemistry*, **2013**, 1022, 82-85	2	26
190	Role of screened exact exchange in accurately describing properties of transition metal oxides: Modeling defects in LaAlO3. *Physical Review B*, **2013**, 88,	3.3	5
189	Testing density functionals for structural phase transitions of solids under pressure: Si, SiO2, and Zr. *Physical Review B*, **2013**, 88,	3.3	74
188	Optical band gap of NpO2 and PuO2 from optical absorbance of epitaxial films. *Journal of Applied Physics*, **2013**, 113, 013515	2.5	42
187	Particle-particle and quasiparticle random phase approximations: connections to coupled cluster theory. *Journal of Chemical Physics*, **2013**, 139, 104113	3.9	60
186	Density functional theory studies of the electronic structure of solid state actinide oxides. *Chemical Reviews*, **2013**, 113, 1063-96	68.1	165

185	Structural phase transitions of the metal oxide perovskites SrTiO3, LaAlO3, and LaTiO3 studied with a screened hybrid functional. *Physical Review B*, **2013**, 87,	3.3	42
184	Assessment of long-range corrected functionals for the prediction of non-linear optical properties of organic materials. *Chemical Physics Letters*, **2013**, 575, 122-125	2.5	53
183	Entanglement and polyradical character of polycyclic aromatic hydrocarbons predicted by projected Hartree-Fock theory. *Journal of Physical Chemistry B*, **2013**, 117, 12750-8	3.4	74
182	On Pair Functions for Strong Correlations. *Journal of Chemical Theory and Computation*, **2013**, 9, 2857-69	6.4	22
181	Excited electronic states from a variational approach based on symmetry-projected Hartree-Fock configurations. *Journal of Chemical Physics*, **2013**, 139, 224110	3.9	26
180	Predicting singlet-triplet energy splittings with projected Hartree-Fock methods. *Journal of Physical Chemistry A*, **2013**, 117, 8073-80	2.8	27
179	Multi-component symmetry-projected approach for molecular ground state correlations. *Journal of Chemical Physics*, **2013**, 139, 204102	3.9	49
178	Capturing static and dynamic correlations by a combination of projected Hartree-Fock and density functional theories. *Journal of Chemical Physics*, **2013**, 138, 134102	3.9	28
177	Multireference symmetry-projected variational approaches for ground and excited states of the one-dimensional Hubbard model. *Physical Review B*, **2013**, 87,	3.3	41
176	Linearized Jastrow-style fluctuations on spin-projected Hartree-Fock. *Journal of Chemical Physics*, **2013**, 139, 234113	3.9	14
175	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. *Physical Review B*, **2013**, 88,	3.3	88
174	Proper and improper zero energy modes in Hartree-Fock theory and their relevance for symmetry breaking and restoration. *Journal of Chemical Physics*, **2013**, 139, 154107	3.9	21
173	N-electron Slater determinants from nonunitary canonical transformations of fermion operators. *Physical Review A*, **2012**, 86,	2.6	12
172	Exploring Copper Oxide Cores Using the Projected Hartree-Fock Method. *Journal of Chemical Theory and Computation*, **2012**, 8, 4944-9	6.4	30
171	Projected Hartree-Fock theory. *Journal of Chemical Physics*, **2012**, 136, 164109	3.9	174
170	Multideterminant Wave Functions in Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2012**, 8, 2181-8	6.4	92
169	Assessment of correlation energies based on the random-phase approximation. *New Journal of Physics*, **2012**, 14, 043002	2.9	111
168	Symmetry-projected variational approach for ground and excited states of the two-dimensional Hubbard model. *Physical Review B*, **2012**, 85,	3.3	38

167	Modeling of the cubic and antiferrodistortive phases of SrTiO3 with screened hybrid density functional theory. *Physical Review B*, **2011**, 84,	3.3	32
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	3.9	32
165	Seniority and orbital symmetry as tools for establishing a full configuration interaction hierarchy. *Journal of Chemical Physics*, **2011**, 135, 044119	3.9	105
164	The indirect to direct band gap transition in multilayered MoS2 as predicted by screened hybrid density functional theory. *Applied Physics Letters*, **2011**, 99, 261908	3.4	431
163	Generalized Hartree-Fock Description of Molecular Dissociation. *Journal of Chemical Theory and Computation*, **2011**, 7, 2667-74	6.4	56
162	Screened hybrid and self-consistent GW calculations of cadmium/magnesium indium sulfide materials. *Physical Review B*, **2011**, 83,	3.3	16
161	Accurate treatment of solids with the HSE screened hybrid. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 767-774	1.3	216
160	Accurate Treatment of Solids with the HSE Screened Hybrid **2011**, 97-110		
159	Projected quasiparticle theory for molecular electronic structure. *Journal of Chemical Physics*, **2011**, 135, 124108	3.9	130
158	5f Electronic Structure and Fermiology of Pu Materials. *Materials Research Society Symposia Proceedings*, **2010**, 1264, 1		3
157	Hybrid functionals including random phase approximation correlation and second-order screened exchange. *Journal of Chemical Physics*, **2010**, 132, 094103	3.9	117
156	Constrained-pairing mean-field theory. III. Inclusion of density functional exchange and correlation effects via alternative densities. *Journal of Chemical Physics*, **2010**, 132, 024111	3.9	28
155	Many-electron self-interaction and spin polarization errors in local hybrid density functionals. *Journal of Chemical Physics*, **2010**, 133, 134116	3.9	78
154	Range-separated local hybrids. *Journal of Chemical Physics*, **2010**, 132, 224106	3.9	34
153	The connection between self-interaction and static correlation: a random phase approximation perspective. *Molecular Physics*, **2010**, 108, 2511-2517	1.7	66
152	Description of magnetic interactions in strongly correlated solids via range-separated hybrid functionals. *Physical Review B*, **2009**, 79,	3.3	41
151	Long-range-corrected hybrid density functionals including random phase approximation correlation: application to noncovalent interactions. *Journal of Chemical Physics*, **2009**, 131, 034110	3.9	78
150	Constrained-pairing mean-field theory. II. Exact treatment of dissociations to nondegenerate orbitals. *Journal of Chemical Physics*, **2009**, 131, 164119	3.9	37

149	Local hybrids as a perturbation to global hybrid functionals. *Journal of Chemical Physics*, **2009**, 131, 154112	3.9	30
148	The role of the reference state in long-range random phase approximation correlation. *Journal of Chemical Physics*, **2009**, 131, 154106	3.9	28
147	Locally range-separated hybrids as linear combinations of range-separated local hybrids. *International Journal of Quantum Chemistry*, **2009**, 109, 2023-2032	2.1	25
146	Strong correlations via constrained-pairing mean-field theory. *Journal of Chemical Physics*, **2009**, 131, 121102	3.9	71
145	Long-Range-Corrected Hybrids Based on a New Model Exchange Hole. *Journal of Chemical Theory and Computation*, **2009**, 5, 754-62	6.4	58
144	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, 11742-9	2.8	48
143	Regularized Gradient Expansion for Atoms, Molecules, and Solids. *Journal of Chemical Theory and Computation*, **2009**, 5, 763-9	6.4	34
142	Coulomb-only second-order perturbation theory in long-range-corrected hybrid density functionals. *Physical Chemistry Chemical Physics*, **2009**, 11, 9677-86	3.6	28
141	MoleculeSurface Orientational Averaging in Surface Enhanced Raman Optical Activity Spectroscopy. *Journal of Physical Chemistry C*, **2009**, 113, 9445-9449	3.8	18
140	Long-range-corrected hybrids including random phase approximation correlation. *Journal of Chemical Physics*, **2009**, 130, 081105	3.9	152
139	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. *Physical Review B*, **2009**, 80,	3.3	42
138	Can short-range hybrids describe long-range-dependent properties?. *Journal of Chemical Physics*, **2009**, 131, 044108	3.9	322
137	Screened hybrid density functionals for solid-state chemistry and physics. *Physical Chemistry Chemical Physics*, **2009**, 11, 443-54	3.6	331
136	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. *Molecular Physics*, **2009**, 107, 1077-1088	1.7	17
135	Generalized gradient approximation model exchange holes for range-separated hybrids. *Journal of Chemical Physics*, **2008**, 128, 194105	3.9	200
134	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. *Physical Review A*, **2008**, 77,	2.6	85
133	Half-metallic graphene nanodots: A comprehensive first-principles theoretical study. *Physical Review B*, **2008**, 77,	3.3	271
132	Accurate solid-state band gaps via screened hybrid electronic structure calculations. *Journal of Chemical Physics*, **2008**, 129, 011102	3.9	140

131	Analytically Calculated Polarizability of Carbon Nanotubes: Single Wall, Coaxial, and Bundled Systems. *Journal of Physical Chemistry C*, **2008**, 112, 1396-1400	3.8	24
130	Resolution of the identity atomic orbital Laplace transformed second order Møller-Plesset theory for nonconducting periodic systems. *Physical Chemistry Chemical Physics*, **2008**, 10, 3421-9	3.6	56
129	Assessment of a Middle-Range Hybrid Functional. *Journal of Chemical Theory and Computation*, **2008**, 4, 1254-62	6.4	135
128	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. *Physical Review A*, **2008**, 78,	2.6	187
127	Hybrid functionals with local range separation. *Journal of Chemical Physics*, **2008**, 129, 124103	3.9	113
126	Self-consistent generalized Kohn-Sham local hybrid functionals of screened exchange: Combining local and range-separated hybridization. *Journal of Chemical Physics*, **2008**, 129, 124110	3.9	59
125	Hartree-Fock orbitals significantly improve the reaction barrier heights predicted by semilocal density functionals. *Journal of Chemical Physics*, **2008**, 128, 244112	3.9	69
124	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. *Physical Review A*, **2008**, 77,	2.6	48
123	Parameterized local hybrid functionals from density-matrix similarity metrics. *Journal of Chemical Physics*, **2008**, 128, 084111	3.9	41
122	Dispersion in the Mott insulator UO2: A comparison of photoemission spectroscopy and screened hybrid density functional theory. *Journal of Computational Chemistry*, **2008**, 29, 2288-94	3.5	56
121	Revisiting the nonlinear optical properties of polybutatriene and polydiacetylene with density functional theory. *Chemical Physics Letters*, **2008**, 456, 101-104	2.5	22
120	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. *Chemical Physics Letters*, **2008**, 465, 226-229	2.5	88
119	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids. *Journal of Chemical Theory and Computation*, **2008**, 4, 123-35	6.4	681
118	The ground state correlation energy of the random phase approximation from a ring coupled cluster doubles approach. *Journal of Chemical Physics*, **2008**, 129, 231101	3.9	239
117	Covalency in the actinide dioxides: Systematic study of the electronic properties using screened hybrid density functional theory. *Physical Review B*, **2007**, 76,	3.3	248
116	Exchange and correlation in open systems of fluctuating electron number. *Physical Review A*, **2007**, 76,	2.6	131
115	Tests of functionals for systems with fractional electron number. *Journal of Chemical Physics*, **2007**, 126, 154109	3.9	503
114	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	3.9	248

113	Noncollinear magnetism in density functional calculations. *Physical Review B*, **2007**, 75,	3.3	67
112	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. *Physical Review A*, **2007**, 76,	2.6	37
111	The importance of middle-range Hartree-Fock-type exchange for hybrid density functionals. *Journal of Chemical Physics*, **2007**, 127, 221103	3.9	139
110	Local hybrid functionals based on density matrix products. *Journal of Chemical Physics*, **2007**, 127, 164117	3.9	53
109	Edge effects in finite elongated graphene nanoribbons. *Physical Review B*, **2007**, 76,	3.3	143
108	Assessment of long-range corrected functionals performance for n-->pi* transitions in organic dyes. *Journal of Chemical Physics*, **2007**, 127, 094102	3.9	112
107	Spurious fractional charge on dissociated atoms: pervasive and resilient self-interaction error of common density functionals. *Journal of Chemical Physics*, **2006**, 125, 194112	3.9	349
106	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,	3.3	119
105	Mott transition of MnO under pressure: A comparison of correlated band theories. *Physical Review B*, **2006**, 74,	3.3	54
104	Importance of short-range versus long-range Hartree-Fock exchange for the performance of hybrid density functionals. *Journal of Chemical Physics*, **2006**, 125, 074106	3.9	747
103	Parametrization of Atomic Energies to Improve Small Basis Set Density Functional Thermochemistry. *Journal of Chemical Theory and Computation*, **2006**, 2, 1045-9	6.4	17
102	Assessment of a long-range corrected hybrid functional. *Journal of Chemical Physics*, **2006**, 125, 234109	3.9	1356
101	Energy storage capacity of polymeric nitrogen. *Molecular Physics*, **2006**, 104, 745-749	1.7	38
100	Theoretical nitrogen NMR chemical shifts in octahedral boron nitride cages. *Journal of Physical Chemistry A*, **2006**, 110, 10844-7	2.8	26
99	Progress in the development of exchange-correlation functionals **2005**, 669-724		96
98	Doping of polyaniline by acid-base chemistry: density functional calculations with periodic boundary conditions. *Journal of the American Chemical Society*, **2005**, 127, 11318-27	16.4	95
97	All-Electron Hybrid Density Functional Calculations on UFn and UCln (n = 1-6). *Journal of Chemical Theory and Computation*, **2005**, 1, 612-6	6.4	31
96	Energy band gaps and lattice parameters evaluated with the Heyd-Scuseria-Ernzerhof screened hybrid functional. *Journal of Chemical Physics*, **2005**, 123, 174101	3.9	1306

95	Assessment of Density Functionals for Predicting One-Bond Carbon-Hydrogen NMR Spin-Spin Coupling Constants. *Journal of Chemical Theory and Computation*, **2005**, 1, 541-5	6.4	63
94	Prescription for the design and selection of density functional approximations: more constraint satisfaction with fewer fits. *Journal of Chemical Physics*, **2005**, 123, 62201	3.9	658
93	Theoretical study of the electronic properties of narrow single-walled carbon nanotubes: beyond the local density approximation. *Journal of Chemical Physics*, **2004**, 121, 10376-9	3.9	52
92	Effect of oxygen chemisorption on the energy band gap of a chiral semiconducting single-walled carbon nanotube. *Chemical Physics Letters*, **2004**, 389, 289-292	2.5	50
91	Nuclear magnetic resonance shielding tensors calculated with kinetic energy density-dependent exchange-correlation functionals. *Chemical Physics Letters*, **2004**, 390, 408-412	2.5	29
90	Meta-generalized gradient approximation: explanation of a realistic nonempirical density functional. *Journal of Chemical Physics*, **2004**, 120, 6898-911	3.9	355
89	Assessment and validation of a screened Coulomb hybrid density functional. *Journal of Chemical Physics*, **2004**, 120, 7274-80	3.9	569
88	Efficient hybrid density functional calculations in solids: assessment of the Heyd-Scuseria-Ernzerhof screened Coulomb hybrid functional. *Journal of Chemical Physics*, **2004**, 121, 1187-92	3.9	1520
87	Climbing the density functional ladder: nonempirical meta-generalized gradient approximation designed for molecules and solids. *Physical Review Letters*, **2003**, 91, 146401	7.4	4737
86	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. *Journal of Chemical Physics*, **2003**, 119, 12129-12137	3.9	1724
85	Hybrid functionals based on a screened Coulomb potential. *Journal of Chemical Physics*, **2003**, 118, 8207-8215	3.9	10573
84	Local hybrid functionals. *Journal of Chemical Physics*, **2003**, 118, 1068-1073	3.9	255
83	Thermodynamics of yield in boron nitride nanotubes. *Physical Review B*, **2003**, 68,	3.3	62
82	A new correlation functional based on a transcorrelated Hamiltonian. *Journal of Chemical Physics*, **2003**, 118, 2464	3.9	22
81	Chalcogenide Exchange Reaction of [RGa(μ-Te)]4 with Elemental Sulfur and Selenium: A Density Functional Theory Study. *Journal of Cluster Science*, **2002**, 13, 587-599	3	4
80	Assessment of simple exchange-correlation energy functionals of the one-particle density matrix. *Journal of Chemical Physics*, **2002**, 117, 2489-2495	3.9	57
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