John P Perdew

List of Publications by Year in Descending Order

188 papers	222,802 citations	67 h-index	195 g-index
195 ext. papers	242,023 ext. citations	5 avg, IF	9.08 L-index

#	Paper	IF	Citations
188	Fermi-Löwdin orbital self-interaction correction of adsorption energies on transition metal ions.. *Journal of Chemical Physics*, **2022**, 156, 134102	3.8	0
187	Construction of meta-GGA functionals through restoration of exact constraint adherence to regularized SCAN functionals.. *Journal of Chemical Physics*, **2022**, 156, 034109	3.8	2
186	Density-related properties from self-interaction corrected density functional theory calculations. *Journal of Chemical Physics*, **2021**, 154, 024102	3.8	4
185	van der Waals corrected density functionals for cylindrical surfaces: Ammonia and nitrogen dioxide adsorbed on a single-walled carbon nanotube. *Physical Review B*, **2021**, 103,	3.3	1
184	Modeling Liquid Water by Climbing up Jacob's Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. *Journal of Physical Chemistry B*, **2021**, 125, 11444-11456	3.3	7
183	Interpretations of ground-state symmetry breaking and strong correlation in wavefunction and density functional theories. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.2	17
182	rSCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. *Journal of Chemical Physics*, **2021**, 154, 061101	3.8	14
181	Self-interaction correction in water-ion clusters. *Journal of Chemical Physics*, **2021**, 154, 094302	3.8	5
180	Exploring and enhancing the accuracy of interior-scaled Perdew-Zunger self-interaction correction. *Journal of Chemical Physics*, **2021**, 154, 094105	3.8	5
179	Spherical vs non-spherical and symmetry-preserving vs symmetry-breaking densities of open-shell atoms in density functional theory.. *Journal of Chemical Physics*, **2021**, 155, 234110	3.8	
178	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. *Nature Communications*, **2021**, 12, 6359	16.9	6
177	Artificial intelligence "sees" split electrons. *Science*, **2021**, 374, 1322-1323	32.2	3
176	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. *Chemical Physics Letters*, **2021**, 780, 138952	2.4	
175	Reimagining the eg1 Electronic State in Oxygen Evolution Catalysis: Oxidation-State-Modulated Superlattices as a New Type of Heterostructure for Maximizing Catalysis. *Advanced Energy Materials*, **2021**, 11, 2101636	21.6	
174	Competing stripe and magnetic phases in the cuprates from first principles. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 68-72	11.2	28
173	Accurate and Numerically Efficient rSCAN Meta-Generalized Gradient Approximation. *Journal of Physical Chemistry Letters*, **2020**, 11, 8208-8215	6.2	53
172	Simple hydrogenic estimates for the exchange and correlation energies of atoms and atomic ions, with implications for density functional theory. *Journal of Chemical Physics*, **2020**, 153, 074114	3.8	3

171	Density functionals combined with van der Waals corrections for graphene adsorbed on layered materials. *Physical Review B*, **2020**, 101,	3.3	4
170	Self-interaction error overbinds water clusters but cancels in structural energy differences. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 11283-11288	11.2	32
169	Constraint-based wave vector and frequency dependent exchange-correlation kernel of the uniform electron gas. *Physical Review B*, **2020**, 101,	3.3	5
168	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. *Journal of Chemical Physics*, **2020**, 152, 214109	3.8	14
167	Hierarchically 3D Porous Ag Nanostructures Derived from Silver Benzenethiolate Nanoboxes: Enabling CO Reduction with a Near-Unity Selectivity and Mass-Specific Current Density over 500 A/g. *Nano Letters*, **2020**, 20, 2806-2811	11.3	25
166	What do we learn from the classical turning surface of the Kohn-Sham potential as electron number is varied continuously?. *Journal of Chemical Physics*, **2020**, 152, 054105	3.8	0
165	Different bonding type along each crystallographic axis: Computational study of poly(p-phenylene terephthalamide). *Physical Review Materials*, **2020**, 4,	3.1	2
164	Simple self-interaction correction to random-phase-approximation-like correlation energies. *Physical Review A*, **2019**, 100,	2.6	6
163	Anisotropic Conductivity at the Single-Molecule Scale. *Angewandte Chemie - International Edition*, **2019**, 58, 14275-14280	16.1	14
162	van der Waals Correction to the Physisorption of Graphene on Metal Surfaces. *Journal of Physical Chemistry C*, **2019**, 123, 13748-13757	3.7	13
161	Stretched or noded orbital densities and self-interaction correction in density functional theory. *Journal of Chemical Physics*, **2019**, 150, 174102	3.8	30
160	Perdew-Zunger self-interaction correction: How wrong for uniform densities and large-Z atoms?. *Journal of Chemical Physics*, **2019**, 150, 174106	3.8	23
159	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-L□wdin self-interaction correction. *Physical Review A*, **2019**, 100,	2.6	23
158	Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors. *Physical Review B*, **2019**, 100,	3.3	25
157	Anisotropic Conductivity at the Single-Molecule Scale. *Angewandte Chemie*, **2019**, 131, 14413-14418	3.5	4
156	Innentitelbild: Anisotropic Conductivity at the Single-Molecule Scale (Angew. Chem. 40/2019). *Angewandte Chemie*, **2019**, 131, 14138-14138	3.5	1
155	Predictive design of intrinsic half-metallicity in zigzag tungsten dichalcogenide nanoribbons. *Physical Review B*, **2019**, 100,	3.3	3
154	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. *Journal of Chemical Physics*, **2019**, 151, 214108	3.8	30

153	First-principles study of the binding energy between nanostructures and its scaling with system size. *Physical Review B*, **2018**, 97,	3.3	12
152	Modeling the physisorption of graphene on metals. *Physical Review B*, **2018**, 97,	3.3	13
151	Accurate critical pressures for structural phase transitions of group IV, III-V, and II-VI compounds from the SCAN density functional. *Physical Review B*, **2018**, 97,	3.3	73
150	Origin of the size-dependence of the equilibrium van der Waals binding between nanostructures. *Journal of Chemical Physics*, **2018**, 148, 074110	3.8	4
149	Efficient first-principles prediction of solid stability: Towards chemical accuracy. *Npj Computational Materials*, **2018**, 4,	10.7	103
148	Collapse of the electron gas from three to two dimensions in Kohn-Sham density functional theory. *Physical Review B*, **2018**, 98,	3.3	5
147	Density-functional energy gaps of solids demystified. *European Physical Journal B*, **2018**, 91, 1	1.2	12
146	Cobalt Intercalated Layered NiFe Double Hydroxides for the Oxygen Evolution Reaction. *Journal of Physical Chemistry B*, **2018**, 122, 847-854	3.3	59
145	Interplay between test sets and statistical procedures in ranking DFT methods: The case of electron density studies. *Mendeleev Communications*, **2018**, 28, 225-235	1.8	26
144	Visualizing atomic sizes and molecular shapes with the classical turning surface of the Kohn-Sham potential. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E11578-E11585	11.2	21
143	How accurate are the parametrized correlation energies of the uniform electron gas?. *Physical Review B*, **2018**, 97,	3.3	6
142	Synergy of van der Waals and self-interaction corrections in transition metal monoxides. *Physical Review B*, **2017**, 96,	3.3	28
141	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. *Physical Review B*, **2017**, 96,	3.3	89
140	Full self-consistency in the Fermi-orbital self-interaction correction. *Physical Review A*, **2017**, 95,	2.6	54
139	Density functional theory is straying from the path toward the exact functional. *Science*, **2017**, 355, 49-52	32.2	522
138	Rehabilitation of the Perdew-Burke-Ernzerhof generalized gradient approximation for layered materials. *Physical Review B*, **2017**, 95,	3.3	52
137	Accuracy of first-principles interatomic interactions and predictions of ferroelectric phase transitions in perovskite oxides: Energy functional and effective Hamiltonian. *Physical Review B*, **2017**, 95,	3.3	30
136	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	11.2	270

135	Response to Comment on "Density functional theory is straying from the path toward the exact functional". *Science*, **2017**, 356, 496	32.2	37
134	Ab initio theory and modeling of water. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 10846-10851	11.2	235
133	Properties of real metallic surfaces: Effects of density functional semilocality and van der Waals nonlocality. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E9188-E9196	11.2	95
132	Redox properties of birnessite from a defect perspective. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 9523-9528	11.2	29
131	Screened van der Waals correction to density functional theory for solids. *Physical Review Materials*, **2017**, 1,	3.1	17
130	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. *Physical Review Letters*, **2016**, 117, 133002	7.3	17
129	Energetics of MnO2 polymorphs in density functional theory. *Physical Review B*, **2016**, 93,	3.3	141
128	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. *Physical Review B*, **2016**, 93,	3.3	127
127	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. *Physical Review X*, **2016**, 6,	9	206
126	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. *Nature Chemistry*, **2016**, 8, 831-6	17.2	456
125	The two pillars: density and spin-density functional theories. *Molecular Physics*, **2016**, 114, 928-931	1.6	6
124	Bending Two-Dimensional Materials To Control Charge Localization and Fermi-Level Shift. *Nano Letters*, **2016**, 16, 2444-9	11.3	56
123	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	1.6	22
122	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. *Journal of Chemical Physics*, **2016**, 144, 191101	3.8	14
121	Semilocal density functionals and constraint satisfaction. *International Journal of Quantum Chemistry*, **2016**, 116, 847-851	2.1	56
120	Water Oxidation Catalyzed by Cobalt Oxide Supported on the Mattagamite Phase of CoTe2. *ACS Catalysis*, **2016**, 6, 7393-7397	12.9	32
119	Paradox of Self-Interaction Correction. *Advances in Atomic, Molecular and Optical Physics*, **2015**, 1-14	1.7	20
118	Semilocal density functional obeying a strongly tightened bound for exchange. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 685-9	11.2	99

117	Van der Waals coefficients beyond the classical shell model. *Journal of Chemical Physics*, **2015**, 142, 024318	3.8	8
116	Strongly Constrained and Appropriately Normed Semilocal Density Functional. *Physical Review Letters*, **2015**, 115, 036402	7.3	1328
115	Gedanken densities and exact constraints in density functional theory. *Journal of Chemical Physics*, **2014**, 140, 18A533	3.8	55
114	Communication: Non-additivity of van der Waals interactions between nanostructures. *Journal of Chemical Physics*, **2014**, 141, 141101	3.8	23
113	Communication: self-interaction correction with unitary invariance in density functional theory. *Journal of Chemical Physics*, **2014**, 140, 121103	3.8	120
112	Density functionals that recognize covalent, metallic, and weak bonds. *Physical Review Letters*, **2013**, 111, 106401	7.3	140
111	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2013**, 9, 355-63	6.2	58
110	Testing density functionals for structural phase transitions of solids under pressure: Si, SiO2, and Zr. *Physical Review B*, **2013**, 88,	3.3	74
109	LONG-RANGE VAN DER WAALS INTERACTION. *International Journal of Modern Physics B*, **2013**, 27, 1330011	1.1	13
108	Climbing the ladder of density functional approximations. *MRS Bulletin*, **2013**, 38, 743-750	3	50
107	Lattice constants from semilocal density functionals with zero-point phonon correction. *Physical Review B*, **2012**, 85,	3.3	53
106	van der Waals interaction as a summable asymptotic series. *Physical Review A*, **2012**, 86,	2.6	15
105	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. *Journal of Physics Condensed Matter*, **2012**, 24, 424207	1.8	12
104	Structural phase transitions in Si and SiO2 crystals via the random phase approximation. *Physical Review B*, **2012**, 86,	3.3	24
103	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. *Physical Review B*, **2011**, 83,	3.3	57
102	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. *Physical Review B*, **2011**, 84,	3.3	135
101	Global Hybrid Functionals: A Look at the Engine under the Hood. *Journal of Chemical Theory and Computation*, **2010**, 6, 3688-3703	6.2	74
100	The RPA Atomization Energy Puzzle. *Journal of Chemical Theory and Computation*, **2010**, 6, 127-34	6.2	70

99	Fourteen easy lessons in density functional theory. *International Journal of Quantum Chemistry*, **2010**, 110, 2801-2807	2.1	36
98	Long-range van der Waals attraction and alkali-metal lattice constants. *Physical Review B*, **2010**, 81,	3.3	61
97	Communication: Ionization potentials in the limit of large atomic number. *Journal of Chemical Physics*, **2010**, 133, 241103	3.8	34
96	Exchange-correlation hole of a generalized gradient approximation for solids and surfaces. *Physical Review B*, **2009**, 79,	3.3	42
95	Comment on Functional derivative of the universal density functional in Fock space *Physical Review A*, **2009**, 79,	2.6	16
94	Density functional theory and the band gap problem. *International Journal of Quantum Chemistry*, **2009**, 28, 497-523	2.1	445
93	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. *Journal of Chemical Theory and Computation*, **2009**, 5, 902-8	6.2	266
92	Workhorse semilocal density functional for condensed matter physics and quantum chemistry. *Physical Review Letters*, **2009**, 103, 026403	7.3	416
91	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. *Molecular Physics*, **2009**, 107, 1077-1088	1.6	17
90	Assessing the performance of recent density functionals for bulk solids. *Physical Review B*, **2009**, 79,	3.3	516
89	Restoring the density-gradient expansion for exchange in solids and surfaces. *Physical Review Letters*, **2008**, 100, 136406	7.3	5732
88	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. *Physical Review A*, **2008**, 77,	2.6	84
87	Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. *Journal of Chemical Theory and Computation*, **2008**, 4, 888-91	6.2	55
86	Simple charge-transfer model to explain the electrical response of hydrogen chains. *Physical Review A*, **2008**, 78,	2.6	19
85	Nonempirical density functionals investigated for jellium: Spin-polarized surfaces, spherical clusters, and bulk linear response. *Physical Review B*, **2008**, 77,	3.3	22
84	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. *Physical Review A*, **2008**, 78,	2.6	180
83	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. *Physical Review A*, **2008**, 77,	2.6	48
82	High-level correlated approach to the jellium surface energy, without uniform-gas input. *Physical Review Letters*, **2008**, 100, 036401	7.3	63

81	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	3.8	244
80	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. *Physical Review A*, **2007**, 76,	2.6	37
79	Uniform Density Limit of Exchange-Correlation Energy Functionals. *ACS Symposium Series*, **2007**, 13-25	0.4	5
78	Exchange and correlation in open systems of fluctuating electron number. *Physical Review A*, **2007**, 76,	2.6	130
77	Spurious fractional charge on dissociated atoms: pervasive and resilient self-interaction error of common density functionals. *Journal of Chemical Physics*, **2006**, 125, 194112	3.8	339
76	Wave-vector analysis of the jellium exchange-correlation surface energy in the random-phase approximation: Support for nonempirical density functionals. *Physical Review B*, **2006**, 74,	3.3	22
75	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. *Journal of Chemical Physics*, **2006**, 124, 94108	3.8	104
74	Relevance of the slowly varying electron gas to atoms, molecules, and solids. *Physical Review Letters*, **2006**, 97, 223002	7.3	82
73	Nonempirical construction of current-density functionals from conventional density-functional approximations. *Physical Review Letters*, **2005**, 95, 196403	7.3	56
72	Binding energy curves from nonempirical density functionals. I. Covalent bonds in closed-shell and radical molecules. *Journal of Physical Chemistry A*, **2005**, 109, 11006-14	2.7	52
71	Prescription for the design and selection of density functional approximations: more constraint satisfaction with fewer fits. *Journal of Chemical Physics*, **2005**, 123, 62201	3.8	645
70	Energies of organic molecules and atoms in density functional theory. *International Journal of Quantum Chemistry*, **2005**, 101, 506-511	2.1	62
69	Energies of isoelectronic atomic ions from a successful metageneralized gradient approximation and other density functionals. *Physical Review A*, **2004**, 70,	2.6	30
68	Spin resolution of the electron-gas correlation energy: Positive same spin contributions. *Physical Review B*, **2004**, 69,	3.3	25
67	Simple physical picture of the Overhauser screened electron-electron interaction. *Physical Review B* , **2004**, 69,	3.3	19
66	Meta-generalized gradient approximation: explanation of a realistic nonempirical density functional. *Journal of Chemical Physics*, **2004**, 120, 6898-911	3.8	353
65	Tests of a ladder of density functionals for bulk solids and surfaces. *Physical Review B*, **2004**, 69,	3.3	307
64	Two avenues to self-interaction correction within Kohn–Sham theory: unitary invariance is the shortcut. *Molecular Physics*, **2003**, 101, 1363-1368	1.6	41

63	Properties of the exchange hole under an appropriate coordinate transformation. *Journal of Chemical Physics*, **2003**, 119, 6457-6464	3.8	24
62	Climbing the density functional ladder: nonempirical meta-generalized gradient approximation designed for molecules and solids. *Physical Review Letters*, **2003**, 91, 146401	7.3	4630
61	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. *Journal of Chemical Physics*, **2003**, 119, 12129-12137	3.8	1666
60	How metals bind: The deformable-jellium model with correlated electrons. *American Journal of Physics*, **2003**, 71, 1048-1061	0.7	8
59	Pair distribution function of the spin-polarized electron gas: A first-principles analytic model for all uniform densities. *Physical Review B*, **2002**, 66,	3.3	70
58	CORRELATION ENERGY DENSITIES: E PLURIBUS UNUM **2002**, 719-730		1
57	Jacob□ ladder of density functional approximations for the exchange-correlation energy. *AIP Conference Proceedings*, **2001**,	0	586
56	EXPLORING THE ADIABATIC CONNECTION BETWEEN WEAK- AND STRONG-INTERACTION LIMITS IN DENSITY FUNCTIONAL THEORY. *International Journal of Modern Physics B*, **2001**, 15, 1672-1683	1.1	6
55	Uniform electron gas from the Colle-Salvetti functional: Missing long-range correlations. *Physical Review A*, **2001**, 63,	2.6	31
54	Short-range correlation in the uniform electron gas: Extended Overhauser model. *Physical Review B* , **2001**, 64,	3.3	65
53	Energy and pressure versus volume: Equations of state motivated by the stabilized jellium model. *Physical Review B*, **2001**, 63,	3.3	116
52	Role of the exchange□orrelation energy: Nature's glue **2000**, 77, 814-818		21
51	How correlation suppresses density fluctuations in the uniform electron gas of one, two, or three dimensions. *International Journal of Quantum Chemistry*, **2000**, 77, 819-830	2.1	37
50	Role of the exchange□orrelation energy: Nature's glue **2000**, 77, 814		1
49	Strictly correlated electrons in density-functional theory. *Physical Review A*, **1999**, 59, 51-54	2.6	123
48	Accurate Density Functional with Correct Formal Properties: A Step Beyond the Generalized Gradient Approximation. *Physical Review Letters*, **1999**, 82, 2544-2547	7.3	603
47	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs **1999**, 75, 889-909		512
46	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs **1999**, 75, 889		15

45	Generalized gradient approximation to the angle- and system-averaged exchange hole. *Journal of Chemical Physics*, **1998**, 109, 3313-3320	3.8	312
44	Why semilocal functionals work: Accuracy of the on-top pair density and importance of system averaging. *Journal of Chemical Physics*, **1998**, 109, 3760-3771	3.8	141
43	Why Density-Gradient Corrections Improve Atomization Energies and Barrier Heights. *Advances in Quantum Chemistry*, **1998**, 33, 1-9	1.4	1
42	Comment on Significance of the highest occupied Kohn-Sham eigenvalue *Physical Review B*, **1997**, 56, 16021-16028	3.3	333
41	Distributions and averages of electron density parameters: Explaining the effects of gradient corrections. *Journal of Chemical Physics*, **1997**, 106, 10184-10193	3.8	127
40	Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. *Physical Review Letters*, **1997**, 78, 1396-1396	7.3	9910
39	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. *International Journal of Quantum Chemistry*, **1997**, 61, 197-205	2.1	85
38	Why the generalized gradient approximation works and how to go beyond it. *International Journal of Quantum Chemistry*, **1997**, 61, 287-293	2.1	106
37	Density-gradient analysis for density functional theory: Application to atoms. *International Journal of Quantum Chemistry*, **1997**, 61, 835-845	2.1	70
36	Correlation entropy of the H2 molecule. *International Journal of Quantum Chemistry*, **1997**, 61, 935-941	2.1	38
35	Coupling-constant dependence of atomization energies. *International Journal of Quantum Chemistry*, **1997**, 64, 285-295	2.1	152
34	Why the generalized gradient approximation works and how to go beyond it **1997**, 61, 287		2
33	Density-gradient analysis for density functional theory: Application to atoms **1997**, 61, 835		3
32	Correlation entropy of the H2 molecule **1997**, 61, 935		5
31	Coupling-constant dependence of atomization energies **1997**, 64, 285		4
30	Coupling-constant dependence of atomization energies **1997**, 64, 285		3
29	Local and Gradient-Corrected Density Functionals. *ACS Symposium Series*, **1996**, 453-462	0.4	48
28	Generalized gradient approximation for the exchange-correlation hole of a many-electron system. *Physical Review B*, **1996**, 54, 16533-16539	3.3	4552

27	Generalized Gradient Approximation Made Simple. *Physical Review Letters*, **1996**, 77, 3865-3868	7.3	117690
26	Rationale for mixing exact exchange with density functional approximations. *Journal of Chemical Physics*, **1996**, 105, 9982-9985	3.8	3780
25	Comparison shopping for a gradient-corrected density functional. *International Journal of Quantum Chemistry*, **1996**, 57, 309-319	2.1	233
24	Self-expansion and compression of charged clusters of stabilized jellium. *International Journal of Quantum Chemistry*, **1996**, 60, 1537-1548	2.1	2
23	Long-range asymptotic behavior of ground-state wave functions, one-matrices, and pair densities. *Journal of Chemical Physics*, **1996**, 105, 2798-2803	3.8	48
22	Comparison shopping for a gradient-corrected density functional **1996**, 57, 309		2
21	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. *Physical Review A*, **1995**, 51, 4531-4541	2.6	308
20	DENSITY FUNCTIONALS AND SMALL INTERPARTICLE SEPARATIONS IN ELECTRONIC SYSTEMS. *Modern Physics Letters B*, **1995**, 09, 829-838	1.5	5
19	Real-space analysis of the exchange-correlation energy. *International Journal of Quantum Chemistry* , **1995**, 56, 199-210	2.1	31
18	Local density and gradient-corrected functionals for short-range correlation: Antiparallel-spin and non-RPA contributions. *International Journal of Quantum Chemistry*, **1993**, 48, 93-100	2.1	30
17	Energetics of small clusters of stabilized jellium: Continuum and shell-structure effects. *International Journal of Quantum Chemistry*, **1993**, 48, 249-261	2.1	22
16	Tight bound and convexity constraint on the exchange-correlation-energy functional in the low-density limit, and other formal tests of generalized-gradient approximations. *Physical Review B*, **1993**, 48, 11638-11645	3.3	142
15	Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. *Physical Review B*, **1992**, 46, 6671-6687	3.3	16979
14	Accurate and simple analytic representation of the electron-gas correlation energy. *Physical Review B*, **1992**, 45, 13244-13249	3.3	19570
13	METAL-SURFACE CORRELATION ENERGY FROM THE LIQUID DROP MODEL: A BACK-OF-THE-ENVELOPE ESTIMATE. *Modern Physics Letters B*, **1991**, 05, 1081-1085	1.5	1
12	Spin scaling of the electron-gas correlation energy in the high-density limit. *Physical Review B*, **1991**, 43, 8911-8916	3.3	279
11	Accurate and simple density functional for the electronic exchange energy: Generalized gradient approximation. *Physical Review B*, **1986**, 33, 8800-8802	3.3	3311
10	Density-functional approximation for the correlation energy of the inhomogeneous electron gas. *Physical Review B*, **1986**, 33, 8822-8824	3.3	15190

9	Success of quantum mechanical approximations for molecular geometries and electron–nuclear attraction expectation values: Gift of the Coulomb potential?. *Journal of Chemical Physics*, **1986**, 84, 4519-4523	3.8	30
8	What do the Kohn-Sham Orbital Energies Mean? How do Atoms Dissociate? **1985**, 265-308		84
7	Accurate Density Functional for the Energy: Real-Space Cutoff of the Gradient Expansion for the Exchange Hole. *Physical Review Letters*, **1985**, 55, 2370-2370	7.3	21
6	Hellmann-Feynman, virial, and scaling requisites for the exact universal density functionals. Shape of the correlation potential and diamagnetic susceptibility for atoms. *Physical Review A*, **1985**, 32, 2010-2021	2.6	800
5	Accurate density functional for the energy: Real-space cutoff of the gradient expansion for the exchange hole. *Physical Review Letters*, **1985**, 55, 1665-1668	7.3	392
4	Density-Functional Theory for Fractional Particle Number: Derivative Discontinuities of the Energy. *Physical Review Letters*, **1982**, 49, 1691-1694	7.3	2184
3	Exchange-correlation energy of a metallic surface: Wave-vector analysis. *Physical Review B*, **1977**, 15, 2884-2901	3.3	817
2	Comparison shopping for a gradient-corrected density functional		4
1	On-top pair-density interpretation of spin density functional theory, with applications to magnetism		1