John P Perdew

List of Publications by Year
in descending order

192 papers	283,292 citations	10389 72 h-index	3323 184 g-index
195 all docs	195 docs citations	195 times ranked	111680 citing authors

#	Article	IF	Citations
1	First-principles wave-vector- and frequency-dependent exchange-correlation kernel for jellium at all densities. Physical Review B, 2022, 105, .	3.2	7
2	Construction of meta-GGA functionals through restoration of exact constraint adherence to regularized SCAN functionals. Journal of Chemical Physics, 2022, 156, 034109.	3.0	25
3	Fermiâ€“LÃ¶wdin orbital self-interaction correction of adsorption energies on transition metal ions. Journal of Chemical Physics, 2022, 156, 134102.	3.0	2
4	How Good Is the Density-Corrected SCAN Functional for Neutral and Ionic Aqueous Systems, and What Is So Right about the Hartreeâ€“Fock Density?. Journal of Chemical Theory and Computation, 2022, 18, 4745-4761.	5.3	20
5	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	3.0	8
6	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, .	7.1	53
7	Calculation and interpretation of classical turning surfaces in solids. Npj Computational Materials, 2021, 7, .	8.7	6
8	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. Journal of Chemical Physics, 2021, 154, 061101.	3.0	70
9	Self-interaction correction in waterâ€“ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	3.0	16
10	Exploring and enhancing the accuracy of interior-scaled Perdewâ€“Zunger self-interaction correction. Journal of Chemical Physics, 2021, 154, 094105.	3.0	12
11	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, .	3.2	2
12	Modeling Liquid Water by Climbing up Jacobâ€™s Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. Journal of Physical Chemistry B, 2021, 125, 11444-11456.	2.6	40
13	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. Chemical Physics Letters, 2021, 780, 138952.	2.6	4
14	Reimagining the e_g¹ Electronic State in Oxygen Evolution Catalysis: Oxidationâ€Stateâ€Modulated Superlattices as a New Type of Heterostructure for Maximizing Catalysis. Advanced Energy Materials, 2021, 11, 2101636.	19.5	6
15	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.	3.0	5
16	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. Nature Communications, 2021, 12, 6359.	12.8	45
17	Artificial intelligence â€œseesâ€•split electrons. Science, 2021, 374, 1322-1323.	12.6	10
18	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.	7.1	61

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19	Accurate and Numerically Efficient r²SCAN Meta-Generalized Gradient Approximation. Journal of Physical Chemistry Letters, 2020, 11, 8208-8215.	4.6	335
20	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.	3.0	10
21	Density functionals combined with van der Waals corrections for graphene adsorbed on layered materials. Physical Review B, 2020, 101, .	3.2	8
22	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.	7.1	57
23	Constraint-based wave vector and frequency dependent exchange-correlation kernel of the uniform electron gas. Physical Review B, 2020, 101, .	3.2	17
24	A step in the direction of resolving the paradox of Perdewâ€“Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. Journal of Chemical Physics, 2020, 152, 214109.	3.0	23
25	Hierarchically 3D Porous Ag Nanostructures Derived from Silver Benzenethiolate Nanoboxes: Enabling CO₂ Reduction with a Near-Unity Selectivity and Mass-Specific Current Density over 500 A/g. Nano Letters, 2020, 20, 2806-2811.	9.1	53
26	What do we learn from the classical turning surface of the Kohnâ€“Sham potential as electron number is varied continuously?. Journal of Chemical Physics, 2020, 152, 054105.	3.0	1
27	Different bonding type along each crystallographic axis: Computational study of poly(p -phenylene) Tj ETQq1 1 0.784314 rgBT /Overlo	2.4	7
28	Perdew-Zunger self-interaction correction: How wrong for uniform densities and large-Z atoms?. Journal of Chemical Physics, 2019, 150, 174106.	3.0	35
29	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-LÃ¶wdin self-interaction correction. Physical Review A, 2019, 100, .	2.5	27
30	Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors. Physical Review B, 2019, 100, .	3.2	44
31	Anisotropic Conductivity at the Singleâ€Molecule Scale. Angewandte Chemie, 2019, 131, 14413-14418.	2.0	6
32	Simple self-interaction correction to random-phase-approximation-like correlation energies. Physical Review A, 2019, 100, .	2.5	13
33	Anisotropic Conductivity at the Singleâ€Molecule Scale. Angewandte Chemie - International Edition, 2019, 58, 14275-14280.	13.8	18
34	van der Waals Correction to the Physisorption of Graphene on Metal Surfaces. Journal of Physical Chemistry C, 2019, 123, 13748-13757.	3.1	18
35	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	3.0	46
36	Innentitelbild: Anisotropic Conductivity at the Singleâ€Molecule Scale (Angew. Chem. 40/2019). Angewandte Chemie, 2019, 131, 14138-14138.	2.0	1

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37	Predictive design of intrinsic half-metallicity in zigzag tungsten dichalcogenide nanoribbons. Physical Review B, 2019, 100, .	3.2	9
38	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. Journal of Chemical Physics, 2019, 151, 214108.	3.0	56
39	First-principles study of the binding energy between nanostructures and its scaling with system size. Physical Review B, 2018, 97, .	3.2	13
40	Modeling the physisorption of graphene on metals. Physical Review B, 2018, 97, .	3.2	15
41	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, .	3.2	100
42	Origin of the size-dependence of the equilibrium van der Waals binding between nanostructures. Journal of Chemical Physics, 2018, 148, 074110.	3.0	39
43	Efficient first-principles prediction of solid stability: Towards chemical accuracy. Npj Computational Materials, 2018, 4, .	8.7	157
44	Cobalt Intercalated Layered NiFe Double Hydroxides for the Oxygen Evolution Reaction. Journal of Physical Chemistry B, 2018, 122, 847-854.	2.6	78
45	Interplay between test sets and statistical procedures in ranking DFT methods: The case of electron density studies. Mendeleev Communications, 2018, 28, 225-235.	1.6	36
46	Visualizing atomic sizes and molecular shapes with the classical turning surface of the Kohnâ€“Sham potential. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E11578-E11585.	7.1	27
47	How accurate are the parametrized correlation energies of the uniform electron gas?. Physical Review B, 2018, 97, .	3.2	16
48	Collapse of the electron gas from three to two dimensions in Kohn-Sham density functional theory. Physical Review B, 2018, 98, .	3.2	11
49	Density-functional energy gaps of solids demystified. European Physical Journal B, 2018, 91, 1.	1.5	15
50	Density functional theory is straying from the path toward the exact functional. Science, 2017, 355, 49-52.	12.6	711
51	Rehabilitation of the Perdew-Burke-Ernzerhof generalized gradient approximation for layered materials. Physical Review B, 2017, 95, .	3.2	91
52	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, .	3.2	51
53	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
54	Response to Comment on â€œDensity functional theory is straying from the path toward the exact functionalâ€• Science, 2017, 356, 496-496.	12.6	51

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55	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	7.1	340
56	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.	7.1	152
57	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.	7.1	50
58	Synergy of van der Waals and self-interaction corrections in transition metal monoxides. Physical Review B, 2017, 96, .	3.2	50
59	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. Physical Review B, 2017, 96, .	3.2	156
60	Full self-consistency in the Fermi-orbital self-interaction correction. Physical Review A, 2017, 95, .	2.5	76
61	Screened van der Waals correction to density functional theory for solids. Physical Review Materials, 2017, 1, .	2.4	19
62	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. Journal of Chemical Physics, 2016, 144, 191101.	3.0	20
63	Semilocal density functionals and constraint satisfaction. International Journal of Quantum Chemistry, 2016, 116, 847-851.	2.0	65
64	Water Oxidation Catalyzed by Cobalt Oxide Supported on the Mattagamite Phase of CoTe₂. ACS Catalysis, 2016, 6, 7393-7397.	11.2	39
65	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. Physical Review Letters, 2016, 117, 133002.	7.8	24
66	Energetics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MnO</mml:mi><mml:mn>2</mml:mn></mml:msub></mm in density functional theory. Physical Review B, 2016, 93, .	3.2	204
67	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. Physical Review B, 2016, 93, .	3.2	182
68	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. Physical Review X, 2016, 6, .	8.9	321
69	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	13.6	698
70	The two pillars: density and spin-density functional theories. Molecular Physics, 2016, 114, 928-931.	1.7	6
71	Bending Two-Dimensional Materials To Control Charge Localization and Fermi-Level Shift. Nano Letters, 2016, 16, 2444-2449.	9.1	74
72	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	23

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73	Strongly Constrained and Appropriately Normed Semilocal Density Functional. Physical Review Letters, 2015, 115, 036402.	7.8	2,273
74	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, 685-689.	7.1	119
75	Van der Waals coefficients beyond the classical shell model. Journal of Chemical Physics, 2015, 142, 024312.	3.0	8
76	Paradox of Self-Interaction Correction. Advances in Atomic, Molecular and Optical Physics, 2015, , 1-14.	2.3	29
77	Gedanken densities and exact constraints in density functional theory. Journal of Chemical Physics, 2014, 140, 18A533.	3.0	82
78	Communication: Non-additivity of van der Waals interactions between nanostructures. Journal of Chemical Physics, 2014, 141, 141101.	3.0	24
79	Communication: Self-interaction correction with unitary invariance in density functional theory. Journal of Chemical Physics, 2014, 140, 121103.	3.0	168
80	LONG-RANGE VAN DER WAALS INTERACTION. International Journal of Modern Physics B, 2013, 27, 1330011.	2.0	14
81	Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. Physical Review Letters, 2013, 111, 106401.	7.8	168
82	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 355-363.	5.3	68
83	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
84	Climbing the ladder of density functional approximations. MRS Bulletin, 2013, 38, 743-750.	3.5	66
85	van der Waals interaction as a summable asymptotic series. Physical Review A, 2012, 86, .	2.5	15
86	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
87	Structural phase transitions in Si and SiO2crystals via the random phase approximation. Physical Review B, 2012, 86, .	3.2	25
88	Lattice constants from semilocal density functionals with zero-point phonon correction. Physical Review B, 2012, 85, .	3.2	63
89	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. Physical Review B, 2011, 84, .	3.2	180
90	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. Physical Review B, 2011, 83, .	3.2	67

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91	Communication: Ionization potentials in the limit of large atomic number. Journal of Chemical Physics, 2010, 133, 241103.	3.0	40
92	Fourteen easy lessons in density functional theory. International Journal of Quantum Chemistry, 2010, 110, 2801-2807.	2.0	41
93	Long-range van der Waals attraction and alkali-metal lattice constants. Physical Review B, 2010, 81, .	3.2	65
94	Global Hybrid Functionals: A Look at the Engine under the Hood. Journal of Chemical Theory and Computation, 2010, 6, 3688-3703.	5.3	87
95	The RPA Atomization Energy Puzzle. Journal of Chemical Theory and Computation, 2010, 6, 127-134.	5.3	76
96	Exchange-correlation hole of a generalized gradient approximation for solids and surfaces. Physical Review B, 2009, 79, .	3.2	54
97	Comment on â€œFunctional derivative of the universal density functional in Fock spaceâ€• Physical Review A, 2009, 79, .	2.5	17
98	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. Journal of Chemical Theory and Computation, 2009, 5, 902-908.	5.3	306
99	Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. Physical Review Letters, 2009, 103, 026403.	7.8	507
100	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. Molecular Physics, 2009, 107, 1077-1088.	1.7	17
101	Assessing the performance of recent density functionals for bulk solids. Physical Review B, 2009, 79, .	3.2	740
102	Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. Physical Review Letters, 2008, 100, 136406.	7.8	8,139
103	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. Physical Review A, 2008, 77, .	2.5	104
104	Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 888-891.	5.3	63
105	Simple charge-transfer model to explain the electrical response of hydrogen chains. Physical Review A, 2008, 78, .	2.5	20
106	Nonempirical density functionals investigated for jellium: Spin-polarized surfaces, spherical clusters, and bulk linear response. Physical Review B, 2008, 77, .	3.2	26
107	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. Physical Review A, 2008, 78, .	2.5	221
108	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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109	High-Level Correlated Approach to the Jellium Surface Energy, without Uniform-Gas Input. Physical Review Letters, 2008, 100, 036401.	7.8	68
110	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
111	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. Physical Review A, 2007, 76, .	2.5	37
112	Uniform Density Limit of Exchange-Correlation Energy Functionals. ACS Symposium Series, 2007, , 13-25.	0.5	5
113	Exchange and correlation in open systems of fluctuating electron number. Physical Review A, 2007, 76, .	2.5	140
114	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. Journal of Chemical Physics, 2006, 124, 094108.	3.0	122
115	Relevance of the Slowly Varying Electron Gas to Atoms, Molecules, and Solids. Physical Review Letters, 2006, 97, 223002.	7.8	94
116	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
117	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, .	3.2	24
118	Energies of organic molecules and atoms in density functional theory. International Journal of Quantum Chemistry, 2005, 101, 506-511.	2.0	64
119	Nonempirical Construction of Current-Density Functionals from Conventional Density-Functional Approximations. Physical Review Letters, 2005, 95, 196403.	7.8	61
120	Binding Energy Curves from Nonempirical Density Functionals. I. Covalent Bonds in Closed-Shell and Radical Molecules. Journal of Physical Chemistry A, 2005, 109, 11006-11014.	2.5	57
121	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
122	Energies of isoelectronic atomic ions from a successful metageneralized gradient approximation and other density functionals. Physical Review A, 2004, 70, .	2.5	33
123	Spin resolution of the electron-gas correlation energy:â€ƒPositive same spin contributions. Physical Review B, 2004, 69, .	3.2	27
124	Simple physical picture of the Overhauser screened electron-electron interaction. Physical Review B, 2004, 69, .	3.2	21
125	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. Journal of Chemical Physics, 2004, 120, 6898-6911.	3.0	431
126	Tests of a ladder of density functionals for bulk solids and surfaces. Physical Review B, 2004, 69, .	3.2	349

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127	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
128	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
129	How metals bind: The deformable-jellium model with correlated electrons. American Journal of Physics, 2003, 71, 1048-1061.	0.7	11
130	Two avenues to self-interaction correction within Kohnâ€”Sham theory: unitary invariance is the shortcut. Molecular Physics, 2003, 101, 1363-1368.	1.7	45
131	Properties of the exchange hole under an appropriate coordinate transformation. Journal of Chemical Physics, 2003, 119, 6457-6464.	3.0	26
132	Pair distribution function of the spin-polarized electron gas:â€ƒA first-principles analytic model for all uniform densities. Physical Review B, 2002, 66, .	3.2	76
133	CORRELATION ENERGY DENSITIES: E PLURIBUS UNUM. , 2002, , 719-730.		1
134	Energy and pressure versus volume: Equations of state motivated by the stabilized jellium model. Physical Review B, 2001, 63, .	3.2	132
135	Jacobâ€™s ladder of density functional approximations for the exchange-correlation energy. AIP Conference Proceedings, 2001, , .	0.4	865
136	EXPLORING THE ADIABATIC CONNECTION BETWEEN WEAK- AND STRONG-INTERACTION LIMITS IN DENSITY FUNCTIONAL THEORY. International Journal of Modern Physics B, 2001, 15, 1672-1683.	2.0	11
137	Uniform electron gas from the Colle-Salvetti functional: Missing long-range correlations. Physical Review A, 2001, 63, .	2.5	31
138	Short-range correlation in the uniform electron gas: Extended Overhauser model. Physical Review B, 2001, 64, .	3.2	72
139	Role of the exchange-correlation energy: Nature's glue. International Journal of Quantum Chemistry, 2000, 77, 814-818.	2.0	32
140	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.	2.0	40
141	Role of the exchangeâ€“correlation energy: Nature's glue. , 2000, 77, 814.		2
142	EXPLORING THE ADIABATIC CONNECTION BETWEEN WEAK- AND STRONG-INTERACTION LIMITS IN DENSITY FUNCTIONAL THEORY. , 2000, , .		0
143	Strictly correlated electrons in density-functional theory. Physical Review A, 1999, 59, 51-54.	2.5	146
144	Accurate Density Functional with Correct Formal Properties: A Step Beyond the Generalized Gradient Approximation. Physical Review Letters, 1999, 82, 2544-2547.	7.8	731

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145	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. International Journal of Quantum Chemistry, 1999, 75, 889-909.	2.0	598
146	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. , 1999, 75, 889.		22
147	Generalized gradient approximation to the angle- and system-averaged exchange hole. Journal of Chemical Physics, 1998, 109, 3313-3320.	3.0	425
148	Why semilocal functionals work: Accuracy of the on-top pair density and importance of system averaging. Journal of Chemical Physics, 1998, 109, 3760-3771.	3.0	167
149	Why Density-Gradient Corrections Improve Atomization Energies and Barrier Heights. Advances in Quantum Chemistry, 1998, 33, 1-9.	0.8	2
150	Comment on â€œSignificance of the highest occupied Kohn-Sham eigenvalueâ€• Physical Review B, 1997, 56, 16021-16028.	3.2	372
151	Distributions and averages of electron density parameters: Explaining the effects of gradient corrections. Journal of Chemical Physics, 1997, 106, 10184-10193.	3.0	144
152	Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. Physical Review Letters, 1997, 78, 1396-1396.	7.8	12,087
153	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. International Journal of Quantum Chemistry, 1997, 61, 197-205.	2.0	97
154	Why the generalized gradient approximation works and how to go beyond it. International Journal of Quantum Chemistry, 1997, 61, 287-293.	2.0	126
155	Density-gradient analysis for density functional theory: Application to atoms. International Journal of Quantum Chemistry, 1997, 61, 835-845.	2.0	81
156	Correlation entropy of the H2 molecule. International Journal of Quantum Chemistry, 1997, 61, 935-941.	2.0	47
157	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	2.0	174
158	Why the generalized gradient approximation works and how to go beyond it. , 1997, 61, 287.		5
159	Density-gradient analysis for density functional theory: Application to atoms. , 1997, 61, 835.		4
160	Correlation entropy of the H2 molecule. , 1997, 61, 935.		7
161	Coupling-constant dependence of atomization energies. , 1997, 64, 285.		4
162	Couplingâ€constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	2.0	3

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163	Local and Gradient-Corrected Density Functionals. ACS Symposium Series, 1996, , 453-462.	0.5	56
164	Generalized gradient approximation for the exchange-correlation hole of a many-electron system. Physical Review B, 1996, 54, 16533-16539.	3.2	5,433
165	Generalized Gradient Approximation Made Simple. Physical Review Letters, 1996, 77, 3865-3868.	7.8	157,044
166	Rationale for mixing exact exchange with density functional approximations. Journal of Chemical Physics, 1996, 105, 9982-9985.	3.0	4,987
167	Comparison shopping for a gradient-corrected density functional. International Journal of Quantum Chemistry, 1996, 57, 309-319.	2.0	276
168	Self-expansion and compression of charged clusters of stabilized jellium. International Journal of Quantum Chemistry, 1996, 60, 1537-1548.	2.0	2
169	Longâ€range asymptotic behavior of groundâ€state wave functions, oneâ€matrices, and pair densities. Journal of Chemical Physics, 1996, 105, 2798-2803.	3.0	51
170	Comparison shopping for a gradientâ€corrected density functional. International Journal of Quantum Chemistry, 1996, 57, 309-319.	2.0	3
171	Real-space analysis of the exchange-correlation energy. International Journal of Quantum Chemistry, 1995, 56, 199-210.	2.0	33
172	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. Physical Review A, 1995, 51, 4531-4541.	2.5	335
173	DENSITY FUNCTIONALS AND SMALL INTERPARTICLE SEPARATIONS IN ELECTRONIC SYSTEMS. Modern Physics Letters B, 1995, 09, 829-838.	1.9	6
174	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.	2.0	32
175	Energetics of small clusters of stabilized jellium: Continuum and shell-structure effects. International Journal of Quantum Chemistry, 1993, 48, 249-261.	2.0	22
176	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.	3.2	159
177	Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. Physical Review B, 1992, 46, 6671-6687.	3.2	19,217
178	Accurate and simple analytic representation of the electron-gas correlation energy. Physical Review B, 1992, 45, 13244-13249.	3.2	22,081
179	Spin scaling of the electron-gas correlation energy in the high-density limit. Physical Review B, 1991, 43, 8911-8916.	3.2	308
180	METAL-SURFACE CORRELATION ENERGY FROM THE LIQUID DROP MODEL: A BACK-OF-THE-ENVELOPE ESTIMATE. Modern Physics Letters B, 1991, 05, 1081-1085.	1.9	1

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181	Accurate and simple density functional for the electronic exchange energy: Generalized gradient approximation. Physical Review B, 1986, 33, 8800-8802.	3.2	3,693
182	Density-functional approximation for the correlation energy of the inhomogeneous electron gas. Physical Review B, 1986, 33, 8822-8824.	3.2	16,966
183	Success of quantum mechanical approximations for molecular geometries and electronâ€“nuclear attraction expectation values: Gift of the Coulomb potential?. Journal of Chemical Physics, 1986, 84, 4519-4523.	3.0	30
184	What do the Kohn-Sham Orbital Energies Mean? How do Atoms Dissociate?. , 1985, , 265-308.		106
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