

# John P Perdew

## List of Publications by Year in descending order

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192  
papers

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#	ARTICLE	IF	CITATIONS
1	Generalized Gradient Approximation Made Simple. <i>Physical Review Letters</i> , 1996, 77, 3865-3868.	2.9	157,044
2	Accurate and simple analytic representation of the electron-gas correlation energy. <i>Physical Review B</i> , 1992, 45, 13244-13249.	1.1	22,081
3	Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. <i>Physical Review B</i> , 1992, 46, 6671-6687.	1.1	19,217
4	Density-functional approximation for the correlation energy of the inhomogeneous electron gas. <i>Physical Review B</i> , 1986, 33, 8822-8824.	1.1	16,966
5	Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. <i>Physical Review Letters</i> , 1997, 78, 1396-1396.	2.9	12,087
6	Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. <i>Physical Review Letters</i> , 2008, 100, 136406.	2.9	8,139
7	Climbing the Density Functional Ladder: Nonempirical Meta-“Generalized Gradient Approximation Designed for Molecules and Solids. <i>Physical Review Letters</i> , 2003, 91, 146401.	2.9	5,673
8	Generalized gradient approximation for the exchange-correlation hole of a many-electron system. <i>Physical Review B</i> , 1996, 54, 16533-16539.	1.1	5,433
9	Rationale for mixing exact exchange with density functional approximations. <i>Journal of Chemical Physics</i> , 1996, 105, 9982-9985.	1.2	4,987
10	Accurate and simple density functional for the electronic exchange energy: Generalized gradient approximation. <i>Physical Review B</i> , 1986, 33, 8800-8802.	1.1	3,693
11	Density-Functional Theory for Fractional Particle Number: Derivative Discontinuities of the Energy. <i>Physical Review Letters</i> , 1982, 49, 1691-1694.	2.9	2,573
12	Strongly Constrained and Appropriately Normed Semilocal Density Functional. <i>Physical Review Letters</i> , 2015, 115, 036402.	2.9	2,273
13	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. <i>Journal of Chemical Physics</i> , 2003, 119, 12129-12137.	1.2	2,157
14	Exchange-correlation energy of a metallic surface: Wave-vector analysis. <i>Physical Review B</i> , 1977, 15, 2884-2901.	1.1	921
15	Hellmann-Feynman, virial, and scaling requisites for the exact universal density functionals. Shape of the correlation potential and diamagnetic susceptibility for atoms. <i>Physical Review A</i> , 1985, 32, 2010-2021.	1.0	897
16	Jacob’s ladder of density functional approximations for the exchange-correlation energy. <i>AIP Conference Proceedings</i> , 2001, . .	0.3	865
17	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. <i>Journal of Chemical Physics</i> , 2005, 123, 062201.	1.2	769
18	Assessing the performance of recent density functionals for bulk solids. <i>Physical Review B</i> , 2009, 79, .	1.1	740

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19	Accurate Density Functional with Correct Formal Properties: A Step Beyond the Generalized Gradient Approximation. <i>Physical Review Letters</i> , 1999, 82, 2544-2547.	2.9	731
20	Density functional theory is straying from the path toward the exact functional. <i>Science</i> , 2017, 355, 49-52.	6.0	711
21	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. <i>Nature Chemistry</i> , 2016, 8, 831-836.	6.6	698
22	Density functional theory and the band gap problem. <i>International Journal of Quantum Chemistry</i> , 1985, 28, 497-523.	1.0	607
23	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. , 1999, 75, 889-909.		598
24	Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. <i>Physical Review Letters</i> , 2009, 103, 026403.	2.9	507
25	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. <i>Journal of Chemical Physics</i> , 2004, 120, 6898-6911.	1.2	431
26	Generalized gradient approximation to the angle- and system-averaged exchange hole. <i>Journal of Chemical Physics</i> , 1998, 109, 3313-3320.	1.2	425
27	Accurate Density Functional for the Energy: Real-Space Cutoff of the Gradient Expansion for the Exchange Hole. <i>Physical Review Letters</i> , 1985, 55, 1665-1668.	2.9	424
28	Understanding band gaps of solids in generalized Kohn-Sham theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 2801-2806.	3.3	423
29	Spurious fractional charge on dissociated atoms: Pervasive and resilient self-interaction error of common density functionals. <i>Journal of Chemical Physics</i> , 2006, 125, 194112.	1.2	383
30	Comment on "Significance of the highest occupied Kohn-Sham eigenvalue". <i>Physical Review B</i> , 1997, 56, 16021-16028.	1.1	372
31	Tests of a ladder of density functionals for bulk solids and surfaces. <i>Physical Review B</i> , 2004, 69, .	1.1	349
32	Ab initio theory and modeling of water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 10846-10851.	3.3	340
33	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. <i>Physical Review A</i> , 1995, 51, 4531-4541.	1.0	335
34	Accurate and Numerically Efficient $r^2$ -SCAN Meta-Generalized Gradient Approximation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8208-8215.	2.1	335
35	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. <i>Physical Review X</i> , 2016, 6, .	2.8	321
36	Spin scaling of the electron-gas correlation energy in the high-density limit. <i>Physical Review B</i> , 1991, 43, 8911-8916.	1.1	308

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37	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 902-908.	2.3	306
38	Comparison shopping for a gradient-corrected density functional. <i>International Journal of Quantum Chemistry</i> , 1996, 57, 309-319.	1.0	276
39	Density functionals that are one- and two- are not always many-electron self-interaction-free, as shown for H <sub>2</sub> <sup>+</sup> , He <sub>2</sub> <sup>+</sup> , LiH <sup>+</sup> , and Ne <sub>2</sub> <sup>+</sup> . <i>Journal of Chemical Physics</i> , 2007, 126, 104102.	1.2	274
40	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. <i>Physical Review A</i> , 2008, 78, .	1.0	221
41	Energetics of $\text{MnO}_2$ in density functional theory. <i>Physical Review B</i> , 2016, 93, .		
42	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. <i>Physical Review B</i> , 2016, 93, .	1.1	182
43	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. <i>Physical Review B</i> , 2011, 84, .	1.1	180
44	Coupling-constant dependence of atomization energies. <i>International Journal of Quantum Chemistry</i> , 1997, 64, 285-295.	1.0	174
45	Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. <i>Physical Review Letters</i> , 2013, 111, 106401.	2.9	168
46	Communication: Self-interaction correction with unitary invariance in density functional theory. <i>Journal of Chemical Physics</i> , 2014, 140, 121103.	1.2	168
47	Why semilocal functionals work: Accuracy of the on-top pair density and importance of system averaging. <i>Journal of Chemical Physics</i> , 1998, 109, 3760-3771.	1.2	167
48	Tight bound and convexity constraint on the exchange-correlation-energy functional in the low-density limit, and other formal tests of generalized-gradient approximations. <i>Physical Review B</i> , 1993, 48, 11638-11645.	1.1	159
49	Efficient first-principles prediction of solid stability: Towards chemical accuracy. <i>Npj Computational Materials</i> , 2018, 4, .	3.5	157
50	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. <i>Physical Review B</i> , 2017, 96, .	1.1	156
51	Properties of real metallic surfaces: Effects of density functional semilocality and van der Waals nonlocality. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E9188-E9196.	3.3	152
52	Strictly correlated electrons in density-functional theory. <i>Physical Review A</i> , 1999, 59, 51-54.	1.0	146
53	Distributions and averages of electron density parameters: Explaining the effects of gradient corrections. <i>Journal of Chemical Physics</i> , 1997, 106, 10184-10193.	1.2	144
54	Exchange and correlation in open systems of fluctuating electron number. <i>Physical Review A</i> , 2007, 76, .	1.0	140

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55	Energy and pressure versus volume: Equations of state motivated by the stabilized jellium model. <i>Physical Review B</i> , 2001, 63, .	1.1	132
56	Why the generalized gradient approximation works and how to go beyond it. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 287-293.	1.0	126
57	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. <i>Journal of Chemical Physics</i> , 2006, 124, 094108.	1.2	122
58	Semilocal density functional obeying a strongly tightened bound for exchange. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 685-689.	3.3	119
59	What do the Kohn-Sham Orbital Energies Mean? How do Atoms Dissociate?. , 1985, , 265-308.		106
60	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. <i>Physical Review A</i> , 2008, 77, .	1.0	104
61	Accurate critical pressures for structural phase transitions of group IV, III-V, and II-VI compounds from the SCAN density functional. <i>Physical Review B</i> , 2018, 97, .	1.1	100
62	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 197-205.	1.0	97
63	Relevance of the Slowly Varying Electron Gas to Atoms, Molecules, and Solids. <i>Physical Review Letters</i> , 2006, 97, 223002.	2.9	94
64	Rehabilitation of the Perdew-Burke-Ernzerhof generalized gradient approximation for layered materials. <i>Physical Review B</i> , 2017, 95, .	1.1	91
65	Global Hybrid Functionals: A Look at the Engine under the Hood. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3688-3703.	2.3	87
66	Testing density functionals for structural phase transitions of solids under pressure: Si, $\text{SiO}_2$ , and Zr. <i>Physical Review B</i> , 2013, 88, .	1.1	87
67	Gedanken densities and exact constraints in density functional theory. <i>Journal of Chemical Physics</i> , 2014, 140, 18A533.	1.2	82
68	Density-gradient analysis for density functional theory: Application to atoms. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 835-845.	1.0	81
69	Cobalt Intercalated Layered NiFe Double Hydroxides for the Oxygen Evolution Reaction. <i>Journal of Physical Chemistry B</i> , 2018, 122, 847-854.	1.2	78
70	Pair distribution function of the spin-polarized electron gas: A first-principles analytic model for all uniform densities. <i>Physical Review B</i> , 2002, 66, .	1.1	76
71	The RPA Atomization Energy Puzzle. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 127-134.	2.3	76
72	Full self-consistency in the Fermi-orbital self-interaction correction. <i>Physical Review A</i> , 2017, 95, .	1.0	76

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73	Bending Two-Dimensional Materials To Control Charge Localization and Fermi-Level Shift. <i>Nano Letters</i> , 2016, 16, 2444-2449.	4.5	74
74	Short-range correlation in the uniform electron gas: Extended Overhauser model. <i>Physical Review B</i> , 2001, 64, .	1.1	72
75	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. <i>Journal of Chemical Physics</i> , 2021, 154, 061101.	1.2	70
76	High-Level Correlated Approach to the Jellium Surface Energy, without Uniform-Gas Input. <i>Physical Review Letters</i> , 2008, 100, 036401.	2.9	68
77	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 355-363.	2.3	68
78	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. <i>Physical Review B</i> , 2011, 83, .	1.1	67
79	Climbing the ladder of density functional approximations. <i>MRS Bulletin</i> , 2013, 38, 743-750.	1.7	66
80	Long-range van der Waals attraction and alkali-metal lattice constants. <i>Physical Review B</i> , 2010, 81, .	1.1	65
81	Semilocal density functionals and constraint satisfaction. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 847-851.	1.0	65
82	Energies of organic molecules and atoms in density functional theory. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 506-511.	1.0	64
83	Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 888-891.	2.3	63
84	Lattice constants from semilocal density functionals with zero-point phonon correction. <i>Physical Review B</i> , 2012, 85, .	1.1	63
85	Nonempirical Construction of Current-Density Functionals from Conventional Density-Functional Approximations. <i>Physical Review Letters</i> , 2005, 95, 196403.	2.9	61
86	Competing stripe and magnetic phases in the cuprates from first principles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 68-72.	3.3	61
87	Binding Energy Curves from Nonempirical Density Functionals. I. Covalent Bonds in Closed-Shell and Radical Molecules. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11006-11014.	1.1	57
88	Self-interaction error overbinds water clusters but cancels in structural energy differences. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 11283-11288.	3.3	57
89	Local and Gradient-Corrected Density Functionals. <i>ACS Symposium Series</i> , 1996, , 453-462.	0.5	56
90	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. <i>Journal of Chemical Physics</i> , 2019, 151, 214108.	1.2	56

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91	Exchange-correlation hole of a generalized gradient approximation for solids and surfaces. <i>Physical Review B</i> , 2009, 79, .	1.1	54
92	Hierarchically 3D Porous Ag Nanostructures Derived from Silver Benzenethiolate Nanoboxes: Enabling CO <sub>2</sub> Reduction with a Near-Unity Selectivity and Mass-Specific Current Density over 500 A/g. <i>Nano Letters</i> , 2020, 20, 2806-2811.	4.5	53
93	Interpretations of ground-state symmetry breaking and strong correlation in wavefunction and density functional theories. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	53
94	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. <i>Physical Review A</i> , 2008, 77, .	1.0	52
95	Long-range asymptotic behavior of ground-state wave functions, one-electron matrices, and pair densities. <i>Journal of Chemical Physics</i> , 1996, 105, 2798-2803.	1.2	51
96	Accuracy of first-principles interatomic interactions and predictions of ferroelectric phase transitions in perovskite oxides: Energy functional and effective Hamiltonian. <i>Physical Review B</i> , 2017, 95, .	1.1	51
97	Response to Comment on "Density functional theory is straying from the path toward the exact functional". <i>Science</i> , 2017, 356, 496-496.	6.0	51
98	Redox properties of birnessite from a defect perspective. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 9523-9528.	3.3	50
99	Synergy of van der Waals and self-interaction corrections in transition metal monoxides. <i>Physical Review B</i> , 2017, 96, .	1.1	50
100	Correlation entropy of the H <sub>2</sub> molecule. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 935-941.	1.0	47
101	Stretched or noded orbital densities and self-interaction correction in density functional theory. <i>Journal of Chemical Physics</i> , 2019, 150, 174102.	1.2	46
102	Two avenues to self-interaction correction within Kohn-Sham theory: unitary invariance is the shortcut. <i>Molecular Physics</i> , 2003, 101, 1363-1368.	0.8	45
103	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. <i>Nature Communications</i> , 2021, 12, 6359.	5.8	45
104	Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors. <i>Physical Review B</i> , 2019, 100, .	1.1	44
105	Fourteen easy lessons in density functional theory. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2801-2807.	1.0	41
106	How correlation suppresses density fluctuations in the uniform electron gas of one, two, or three dimensions. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 819-830.	1.0	40
107	Communication: Ionization potentials in the limit of large atomic number. <i>Journal of Chemical Physics</i> , 2010, 133, 241103.	1.2	40
108	Modeling Liquid Water by Climbing up Jacob's Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11444-11456.	1.2	40

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109	Water Oxidation Catalyzed by Cobalt Oxide Supported on the Mattagamite Phase of $\text{CoTe}_2$ . ACS Catalysis, 2016, 6, 7393-7397.	5.5	39
110	Origin of the size-dependence of the equilibrium van der Waals binding between nanostructures. Journal of Chemical Physics, 2018, 148, 074110.	1.2	39
111	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. Physical Review A, 2007, 76, .	1.0	37
112	Interplay between test sets and statistical procedures in ranking DFT methods: The case of electron density studies. Mendeleev Communications, 2018, 28, 225-235.	0.6	36
113	Perdew-Zunger self-interaction correction: How wrong for uniform densities and large- $Z$ atoms?. Journal of Chemical Physics, 2019, 150, 174106.	1.2	35
114	Real-space analysis of the exchange-correlation energy. International Journal of Quantum Chemistry, 1995, 56, 199-210.	1.0	33
115	Energies of isoelectronic atomic ions from a successful metageneralized gradient approximation and other density functionals. Physical Review A, 2004, 70, .	1.0	33
116	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.	1.0	32
117	Role of the exchange-correlation energy: Nature's glue. , 2000, 77, 814-818.		32
118	Uniform electron gas from the Colle-Salvetti functional: Missing long-range correlations. Physical Review A, 2001, 63, .	1.0	31
119	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.	1.2	30
120	Paradox of Self-Interaction Correction. Advances in Atomic, Molecular and Optical Physics, 2015, , 1-14.	2.3	29
121	Spin resolution of the electron-gas correlation energy: Positive same spin contributions. Physical Review B, 2004, 69, .	1.1	27
122	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.	3.3	27
123	Self-interaction-free electric dipole polarizabilities for atoms and their ions using the Fermi-Löwdin self-interaction correction. Physical Review A, 2019, 100, .	1.0	27
124	Properties of the exchange hole under an appropriate coordinate transformation. Journal of Chemical Physics, 2003, 119, 6457-6464.	1.2	26
125	Nonempirical density functionals investigated for jellium: Spin-polarized surfaces, spherical clusters, and bulk linear response. Physical Review B, 2008, 77, .	1.1	26
126	Structural phase transitions in Si and $\text{SiO}_2$ crystals via the random phase approximation. Physical Review B, 2012, 86, .	1.1	25



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127	Construction of meta-GGA functionals through restoration of exact constraint adherence to regularized SCAN functionals. <i>Journal of Chemical Physics</i> , 2022, 156, 034109.	1.2	25
128	Wave-vector analysis of the jellium exchange-correlation surface energy in the random-phase approximation: Support for nonempirical density functionals. <i>Physical Review B</i> , 2006, 74, .	1.1	24
129	Communication: Non-additivity of van der Waals interactions between nanostructures. <i>Journal of Chemical Physics</i> , 2014, 141, 141101.	1.2	24
130	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. <i>Physical Review Letters</i> , 2016, 117, 133002.	2.9	24
131	Accurate Density Functional for the Energy: Real-Space Cutoff of the Gradient Expansion for the Exchange Hole. <i>Physical Review Letters</i> , 1985, 55, 2370-2370.	2.9	23
132	Combinations of coupled cluster, density functionals, and the random phase approximation for describing static and dynamic correlation, and van der Waals interactions. <i>Molecular Physics</i> , 2016, 114, 997-1018.	0.8	23
133	A step in the direction of resolving the paradox of Perdew's Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. <i>Journal of Chemical Physics</i> , 2020, 152, 214109.	1.2	23
134	Energetics of small clusters of stabilized jellium: Continuum and shell-structure effects. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 249-261.	1.0	22
135	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. , 1999, 75, 889.		22
136	Simple physical picture of the Overhauser screened electron-electron interaction. <i>Physical Review B</i> , 2004, 69, .	1.1	21
137	Simple charge-transfer model to explain the electrical response of hydrogen chains. <i>Physical Review A</i> , 2008, 78, .	1.0	20
138	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. <i>Journal of Chemical Physics</i> , 2016, 144, 191101.	1.2	20
139	How Good Is the Density-Corrected SCAN Functional for Neutral and Ionic Aqueous Systems, and What Is So Right about the Hartree-Fock Density?. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4745-4761.	2.3	20
140	Screened van der Waals correction to density functional theory for solids. <i>Physical Review Materials</i> , 2017, 1, .	0.9	19
141	Anisotropic Conductivity at the Single-Molecule Scale. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 14275-14280.	7.2	18
142	van der Waals Correction to the Physisorption of Graphene on Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13748-13757.	1.5	18
143	Comment on "Functional derivative of the universal density functional in Fock space". <i>Physical Review A</i> , 2009, 79, .	1.0	17
144	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. <i>Molecular Physics</i> , 2009, 107, 1077-1088.	0.8	17

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145	Constraint-based wave vector and frequency dependent exchange-correlation kernel of the uniform electron gas. <i>Physical Review B</i> , 2020, 101, .	1.1	17
146	How accurate are the parametrized correlation energies of the uniform electron gas?. <i>Physical Review B</i> , 2018, 97, .	1.1	16
147	Self-interaction correction in water <sup>+</sup> ion clusters. <i>Journal of Chemical Physics</i> , 2021, 154, 094302.	1.2	16
148	van der Waals interaction as a summable asymptotic series. <i>Physical Review A</i> , 2012, 86, .	1.0	15
149	Modeling the physisorption of graphene on metals. <i>Physical Review B</i> , 2018, 97, .	1.1	15
150	Density-functional energy gaps of solids demystified. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	15
151	LONG-RANGE VAN DER WAALS INTERACTION. <i>International Journal of Modern Physics B</i> , 2013, 27, 1330011.	1.0	14
152	First-principles study of the binding energy between nanostructures and its scaling with system size. <i>Physical Review B</i> , 2018, 97, .	1.1	13
153	Simple self-interaction correction to random-phase-approximation-like correlation energies. <i>Physical Review A</i> , 2019, 100, .	1.0	13
154	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 424207.	0.7	12
155	Exploring and enhancing the accuracy of interior-scaled Perdew <sup>+</sup> Zunger self-interaction correction. <i>Journal of Chemical Physics</i> , 2021, 154, 094105.	1.2	12
156	EXPLORING THE ADIABATIC CONNECTION BETWEEN WEAK- AND STRONG-INTERACTION LIMITS IN DENSITY FUNCTIONAL THEORY. <i>International Journal of Modern Physics B</i> , 2001, 15, 1672-1683.	1.0	11
157	How metals bind: The deformable-jellium model with correlated electrons. <i>American Journal of Physics</i> , 2003, 71, 1048-1061.	0.3	11
158	Collapse of the electron gas from three to two dimensions in Kohn-Sham density functional theory. <i>Physical Review B</i> , 2018, 98, .	1.1	11
159	Simple hydrogenic estimates for the exchange and correlation energies of atoms and atomic ions, with implications for density functional theory. <i>Journal of Chemical Physics</i> , 2020, 153, 074114.	1.2	10
160	Artificial intelligence <sup>+</sup> split electrons. <i>Science</i> , 2021, 374, 1322-1323.	6.0	10
161	Predictive design of intrinsic half-metallicity in zigzag tungsten dichalcogenide nanoribbons. <i>Physical Review B</i> , 2019, 100, .	1.1	9
162	Van der Waals coefficients beyond the classical shell model. <i>Journal of Chemical Physics</i> , 2015, 142, 024312.	1.2	8

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163	Density functionals combined with van der Waals corrections for graphene adsorbed on layered materials. <i>Physical Review B</i> , 2020, 101, .	1.1	8
164	Density-related properties from self-interaction corrected density functional theory calculations. <i>Journal of Chemical Physics</i> , 2021, 154, 024102.	1.2	8
165	Correlation entropy of the H <sub>2</sub> molecule. , 1997, 61, 935.		7
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