John P Perdew

List of Publications by Year in descending order

192 papers	283,292 citations	10956 71 h-index	3563 181 g-index
195 all docs	195 docs citations	195 times ranked	111680 citing authors

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

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19	Accurate Density Functional with Correct Formal Properties: A Step Beyond the Generalized Gradient Approximation. Physical Review Letters, 1999, 82, 2544-2547.	2.9	731
20	Density functional theory is straying from the path toward the exact functional. Science, 2017, 355, 49-52.	6.0	711
21	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	6.6	698
22	Density functional theory and the band gap problem. International Journal of Quantum Chemistry, 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. Physical Review Letters, 2009, 103, 026403.	2.9	507
25	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. Journal of Chemical Physics, 2004, 120, 6898-6911.	1.2	431
26	Generalized gradient approximation to the angle- and system-averaged exchange hole. Journal of Chemical Physics, 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. Physical Review Letters, 1985, 55, 1665-1668.	2.9	424
28	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.	3.3	423
29	Spurious fractional charge on dissociated atoms: Pervasive and resilient self-interaction error of common density functionals. Journal of Chemical Physics, 2006, 125, 194112.	1.2	383
30	Comment on â€œSignificance of the highest occupied Kohn-Sham eigenvalueâ€• Physical Review B, 1997, 56, 16021-16028.	1.1	372
31	Tests of a ladder of density functionals for bulk solids and surfaces. Physical Review B, 2004, 69, .	1.1	349
32	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	3.3	340
33	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. Physical Review A, 1995, 51, 4531-4541.	1.0	335
34	Accurate and Numerically Efficient r²SCAN Meta-Generalized Gradient Approximation. Journal of Physical Chemistry Letters, 2020, 11, 8208-8215.	2.1	335
35	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. Physical Review X, 2016, 6, .	2.8	321
36	Spin scaling of the electron-gas correlation energy in the high-density limit. Physical Review B, 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. Journal of Chemical Theory and Computation, 2009, 5, 902-908.	2.3	306
38	Comparison shopping for a gradient-corrected density functional. International Journal of Quantum Chemistry, 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 H2+, He2+, LiH+, and Ne2+. Journal of Chemical Physics, 2007, 126, 104102.	1.2	274
40	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. Physical Review A, 2008, 78, .	1.0	221
41	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></mml in density functional theory. Physical Review B, 2016, 93, .	1.1	204
42	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. Physical Review B, 2016, 93, .	1.1	182
43	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. Physical Review B, 2011, 84, .	1.1	180
44	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	1.0	174
45	Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. Physical Review Letters, 2013, 111, 106401.	2.9	168
46	Communication: Self-interaction correction with unitary invariance in density functional theory. Journal of Chemical Physics, 2014, 140, 121103.	1.2	168
47	Why semilocal functionals work: Accuracy of the on-top pair density and importance of system averaging. Journal of Chemical Physics, 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. Physical Review B, 1993, 48, 11638-11645.	1.1	159
49	Efficient first-principles prediction of solid stability: Towards chemical accuracy. Npj Computational Materials, 2018, 4, .	3.5	157
50	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. Physical Review B, 2017, 96, .	1.1	156
51	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.	3.3	152
52	Strictly correlated electrons in density-functional theory. Physical Review A, 1999, 59, 51-54.	1.0	146
53	Distributions and averages of electron density parameters: Explaining the effects of gradient corrections. Journal of Chemical Physics, 1997, 106, 10184-10193.	1.2	144
54	Exchange and correlation in open systems of fluctuating electron number. Physical Review A, 2007, 76, .	1.0	140

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55	Energy and pressure versus volume: Equations of state motivated by the stabilized jellium model. Physical Review B, 2001, 63, .	1.1	132
56	Why the generalized gradient approximation works and how to go beyond it. International Journal of Quantum Chemistry, 1997, 61, 287-293.	1.0	126
57	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. Journal of Chemical Physics, 2006, 124, 094108.	1.2	122
58	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.	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. Physical Review A, 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. Physical Review B, 2018, 97, .	1.1	100
62	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. International Journal of Quantum Chemistry, 1997, 61, 197-205.	1.0	97
63	Relevance of the Slowly Varying Electron Gas to Atoms, Molecules, and Solids. Physical Review Letters, 2006, 97, 223002.	2.9	94
64	Rehabilitation of the Perdew-Burke-Ernzerhof generalized gradient approximation for layered materials. Physical Review B, 2017, 95, .	1.1	91
65	Global Hybrid Functionals: A Look at the Engine under the Hood. Journal of Chemical Theory and Computation, 2010, 6, 3688-3703.	2.3	87
66	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, .	1.1	87
67	Gedanken densities and exact constraints in density functional theory. Journal of Chemical Physics, 2014, 140, 18A533.	1.2	82
68	Density-gradient analysis for density functional theory: Application to atoms. International Journal of Quantum Chemistry, 1997, 61, 835-845.	1.0	81
69	Cobalt Intercalated Layered NiFe Double Hydroxides for the Oxygen Evolution Reaction. Journal of Physical Chemistry B, 2018, 122, 847-854.	1.2	78
70	Pair distribution function of the spin-polarized electron gas:â€ƒA first-principles analytic model for all uniform densities. Physical Review B, 2002, 66, .	1.1	76
71	The RPA Atomization Energy Puzzle. Journal of Chemical Theory and Computation, 2010, 6, 127-134.	2.3	76
72	Full self-consistency in the Fermi-orbital self-interaction correction. Physical Review A, 2017, 95, .	1.0	76

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

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91	Exchange-correlation hole of a generalized gradient approximation for solids and surfaces. Physical Review B, 2009, 79, .	1.1	54
92	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.	4.5	53
93	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, .	3.3	53
94	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. Physical Review A, 2008, 77, .	1.0	52
95	Longâ€range asymptotic behavior of groundâ€state wave functions, oneâ€matrices, and pair densities. Journal of Chemical Physics, 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. Physical Review B, 2017, 95, .	1.1	51
97	Response to Comment on â€œDensity functional theory is straying from the path toward the exact functionalâ€• Science, 2017, 356, 496-496.	6.0	51
98	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.	3.3	50
99	Synergy of van der Waals and self-interaction corrections in transition metal monoxides. Physical Review B, 2017, 96, .	1.1	50
100	Correlation entropy of the H2 molecule. International Journal of Quantum Chemistry, 1997, 61, 935-941.	1.0	47
101	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	1.2	46
102	Two avenues to self-interaction correction within Kohnâ€”Sham theory: unitary invariance is the shortcut. Molecular Physics, 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. Nature Communications, 2021, 12, 6359.	5.8	45
104	Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors. Physical Review B, 2019, 100, .	1.1	44
105	Fourteen easy lessons in density functional theory. International Journal of Quantum Chemistry, 2010, 110, 2801-2807.	1.0	41
106	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.	1.0	40
107	Communication: Ionization potentials in the limit of large atomic number. Journal of Chemical Physics, 2010, 133, 241103.	1.2	40
108	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.	1.2	40

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109	Water Oxidation Catalyzed by Cobalt Oxide Supported on the Mattagamite Phase of CoTe₂. 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 electronâ€“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:â€ƒPositive 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 Kohnâ€“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-LÃ¶wdin 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 SiO2crystals 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. Journal of Chemical Physics, 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. Physical Review B, 2006, 74, .	1.1	24
129	Communication: Non-additivity of van der Waals interactions between nanostructures. Journal of Chemical Physics, 2014, 141, 141101.	1.2	24
130	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. Physical Review Letters, 2016, 117, 133002.	2.9	24
131	Accurate Density Functional for the Energy: Real-Space Cutoff of the Gradient Expansion for the Exchange Hole. Physical Review Letters, 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. Molecular Physics, 2016, 114, 997-1018.	0.8	23
133	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.	1.2	23
134	Energetics of small clusters of stabilized jellium: Continuum and shell-structure effects. International Journal of Quantum Chemistry, 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. Physical Review B, 2004, 69, .	1.1	21
137	Simple charge-transfer model to explain the electrical response of hydrogen chains. Physical Review A, 2008, 78, .	1.0	20
138	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. Journal of Chemical Physics, 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 Hartreeâ€“Fock Density?. Journal of Chemical Theory and Computation, 2022, 18, 4745-4761.	2.3	20
140	Screened van der Waals correction to density functional theory for solids. Physical Review Materials, 2017, 1, .	0.9	19
141	Anisotropic Conductivity at the Singleâ€Molecule Scale. Angewandte Chemie - International Edition, 2019, 58, 14275-14280.	7.2	18
142	van der Waals Correction to the Physisorption of Graphene on Metal Surfaces. Journal of Physical Chemistry C, 2019, 123, 13748-13757.	1.5	18
143	Comment on â€œFunctional derivative of the universal density functional in Fock spaceâ€. Physical Review A, 2009, 79, .	1.0	17
144	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. Molecular Physics, 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. Physical Review B, 2020, 101, .	1.1	17
146	How accurate are the parametrized correlation energies of the uniform electron gas?. Physical Review B, 2018, 97, .	1.1	16
147	Self-interaction correction in waterâ€“ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	1.2	16
148	van der Waals interaction as a summable asymptotic series. Physical Review A, 2012, 86, .	1.0	15
149	Modeling the physisorption of graphene on metals. Physical Review B, 2018, 97, .	1.1	15
150	Density-functional energy gaps of solids demystified. European Physical Journal B, 2018, 91, 1.	0.6	15
151	LONG-RANGE VAN DER WAALS INTERACTION. International Journal of Modern Physics B, 2013, 27, 1330011.	1.0	14
152	First-principles study of the binding energy between nanostructures and its scaling with system size. Physical Review B, 2018, 97, .	1.1	13
153	Simple self-interaction correction to random-phase-approximation-like correlation energies. Physical Review A, 2019, 100, .	1.0	13
154	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. Journal of Physics Condensed Matter, 2012, 24, 424207.	0.7	12
155	Exploring and enhancing the accuracy of interior-scaled Perdewâ€“Zunger self-interaction correction. Journal of Chemical Physics, 2021, 154, 094105.	1.2	12
156	EXPLORING THE ADIABATIC CONNECTION BETWEEN WEAK- AND STRONG-INTERACTION LIMITS IN DENSITY FUNCTIONAL THEORY. International Journal of Modern Physics B, 2001, 15, 1672-1683.	1.0	11
157	How metals bind: The deformable-jellium model with correlated electrons. American Journal of Physics, 2003, 71, 1048-1061.	0.3	11
158	Collapse of the electron gas from three to two dimensions in Kohn-Sham density functional theory. Physical Review B, 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. Journal of Chemical Physics, 2020, 153, 074114.	1.2	10
160	Artificial intelligence â€œseesâ€•split electrons. Science, 2021, 374, 1322-1323.	6.0	10
161	Predictive design of intrinsic half-metallicity in zigzag tungsten dichalcogenide nanoribbons. Physical Review B, 2019, 100, .	1.1	9
162	Van der Waals coefficients beyond the classical shell model. Journal of Chemical Physics, 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. Physical Review B, 2020, 101, .	1.1	8
164	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	1.2	8
165	Correlation entropy of the H2 molecule. , 1997, 61, 935.		7
166	Different bonding type along each crystallographic axis: Computational study of poly(p -phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.9	7
167	First-principles wave-vector- and frequency-dependent exchange-correlation kernel for jellium at all densities. Physical Review B, 2022, 105, .	1.1	7
168	DENSITY FUNCTIONALS AND SMALL INTERPARTICLE SEPARATIONS IN ELECTRONIC SYSTEMS. Modern Physics Letters B, 1995, 09, 829-838.	1.0	6
169	The two pillars: density and spin-density functional theories. Molecular Physics, 2016, 114, 928-931.	0.8	6
170	Anisotropic Conductivity at the Singleâ€Molecule Scale. Angewandte Chemie, 2019, 131, 14413-14418.	1.6	6
171	Calculation and interpretation of classical turning surfaces in solids. Npj Computational Materials, 2021, 7, .	3.5	6
172	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.	10.2	6
173	Uniform Density Limit of Exchange-Correlation Energy Functionals. ACS Symposium Series, 2007, , 13-25.	0.5	5
174	Comparison shopping for a gradient-corrected density functional. , 0, .		5
175	Why the generalized gradient approximation works and how to go beyond it. , 1997, 61, 287.		5
176	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.	1.2	5
177	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. Chemical Physics Letters, 2021, 780, 138952.	1.2	4
178	Density-gradient analysis for density functional theory: Application to atoms. , 1997, 61, 835.		4
179	Coupling-constant dependence of atomization energies. , 1997, 64, 285.		4
180	Comparison shopping for a gradient-corrected density functional. , 1996, 57, 309.		3

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181	On-top pair-density interpretation of spin density functional theory, with applications to magnetism. , 0, .		3
182	Couplingâ€constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	1.0	3
183	Self-expansion and compression of charged clusters of stabilized jellium. International Journal of Quantum Chemistry, 1996, 60, 1537-1548.	1.0	2
184	Why Density-Gradient Corrections Improve Atomization Energies and Barrier Heights. Advances in Quantum Chemistry, 1998, 33, 1-9.	0.4	2
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, .	1.1	2
186	Role of the exchangeâ€“correlation energy: Nature's glue. , 2000, 77, 814.		2
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