John P Perdew

List of Publications by Year
in descending order

197 papers	296,384 citations	9878 73 h-index	2476 196 g-index
212 all docs	212 docs citations	212 times ranked	144088 citing authors

#	Article	IF	Citations
1	Generalized Gradient Approximation Made Simple. Physical Review Letters, 1996, 77, 3865-3868.	8.0	165,707
2	Accurate and simple analytic representation of the electron-gas correlation energy. Physical Review B, 1992, 45, 13244-13249.	3.3	22,506
3	Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. Physical Review B, 1992, 46, 6671-6687.	3.3	19,704
4	Density-functional approximation for the correlation energy of the inhomogeneous electron gas. Physical Review B, 1986, 33, 8822-8824.	3.3	17,251
5	Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. Physical Review Letters, 1997, 78, 1396-1396.	8.0	12,486
6	Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. Physical Review Letters, 2008, 100, 136406.	8.0	8,703
7	Climbing the Density Functional Ladder: Nonempirical Metaâ€“Generalized Gradient Approximation Designed for Molecules and Solids. Physical Review Letters, 2003, 91, 146401.	8.0	5,861
8	Generalized gradient approximation for the exchange-correlation hole of a many-electron system. Physical Review B, 1996, 54, 16533-16539.	3.3	5,632
9	Rationale for mixing exact exchange with density functional approximations. Journal of Chemical Physics, 1996, 105, 9982-9985.	3.1	5,259
10	Accurate and simple density functional for the electronic exchange energy: Generalized gradient approximation. Physical Review B, 1986, 33, 8800-8802.	3.3	3,783
11	Density-Functional Theory for Fractional Particle Number: Derivative Discontinuities of the Energy. Physical Review Letters, 1982, 49, 1691-1694.	8.0	2,648
12	Strongly Constrained and Appropriately Normed Semilocal Density Functional. Physical Review Letters, 2015, 115, 036402.	8.0	2,483
13	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2003, 119, 12129-12137.	3.1	2,259
14	Exchange-correlation energy of a metallic surface: Wave-vector analysis. Physical Review B, 1977, 15, 2884-2901.	3.3	941
15	Jacobâ€™s ladder of density functional approximations for the exchange-correlation energy. AIP Conference Proceedings, 2001, , .	1.0	920
16	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.	2.5	906
17	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. Journal of Chemical Physics, 2005, 123, 062201.	3.1	795
18	Assessing the performance of recent density functionals for bulk solids. Physical Review B, 2009, 79, .	3.3	773

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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.	8.0	753
20	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	14.3	744
21	Density functional theory and the band gap problem. International Journal of Quantum Chemistry, 1985, 28, 497-523.	2.1	640
22	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. International Journal of Quantum Chemistry, 1999, 75, 889-909.	2.1	609
23	Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. Physical Review Letters, 2009, 103, 026403.	8.0	527
24	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. Journal of Chemical Physics, 2004, 120, 6898-6911.	3.1	463
25	Accurate and Numerically Efficient r²SCAN Meta-Generalized Gradient Approximation. Journal of Physical Chemistry Letters, 2020, 11, 8208-8215.	4.9	463
26	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.	7.6	447
27	Generalized gradient approximation to the angle- and system-averaged exchange hole. Journal of Chemical Physics, 1998, 109, 3313-3320.	3.1	444
28	Accurate Density Functional for the Energy: Real-Space Cutoff of the Gradient Expansion for the Exchange Hole. Physical Review Letters, 1985, 55, 1665-1668.	8.0	437
29	Spurious fractional charge on dissociated atoms: Pervasive and resilient self-interaction error of common density functionals. Journal of Chemical Physics, 2006, 125, 194112.	3.1	390
30	Comment on â€œSignificance of the highest occupied Kohn-Sham eigenvalueâ€• Physical Review B, 1997, 56, 16021-16028.	3.3	381
31	Tests of a ladder of density functionals for bulk solids and surfaces. Physical Review B, 2004, 69, .	3.3	355
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.	7.6	354
33	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. Physical Review X, 2016, 6, .	9.1	344
34	Escaping the symmetry dilemma through a pair-density interpretation of spin-density functional theory. Physical Review A, 1995, 51, 4531-4541.	2.5	339
35	Spin scaling of the electron-gas correlation energy in the high-density limit. Physical Review B, 1991, 43, 8911-8916.	3.3	311
36	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. Journal of Chemical Theory and Computation, 2009, 5, 902-908.	5.6	310

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37	Comparison shopping for a gradient-corrected density functional. International Journal of Quantum Chemistry, 1996, 57, 309-319.	2.1	282
38	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.	3.1	277
39	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. Physical Review A, 2008, 78, .	2.5	228
40	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, .	3.3	214
41	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. Physical Review B, 2016, 93, .	3.3	190
42	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. Physical Review B, 2011, 84, .	3.3	185
43	Communication: Self-interaction correction with unitary invariance in density functional theory. Journal of Chemical Physics, 2014, 140, 121103.	3.1	176
44	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	2.1	175
45	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. Physical Review B, 2017, 96, .	3.3	174
46	Why semilocal functionals work: Accuracy of the on-top pair density and importance of system averaging. Journal of Chemical Physics, 1998, 109, 3760-3771.	3.1	170
47	Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. Physical Review Letters, 2013, 111, 106401.	8.0	170
48	Efficient first-principles prediction of solid stability: Towards chemical accuracy. Npj Computational Materials, 2018, 4, .	9.1	166
49	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	160
50	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.	7.6	159
51	Strictly correlated electrons in density-functional theory. Physical Review A, 1999, 59, 51-54.	2.5	156
52	Distributions and averages of electron density parameters: Explaining the effects of gradient corrections. Journal of Chemical Physics, 1997, 106, 10184-10193.	3.1	144
53	Exchange and correlation in open systems of fluctuating electron number. Physical Review A, 2007, 76, .	2.5	140
54	Energy and pressure versus volume: Equations of state motivated by the stabilized jellium model. Physical Review B, 2001, 63, .	3.3	134

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55	Why the generalized gradient approximation works and how to go beyond it. International Journal of Quantum Chemistry, 1997, 61, 287-293.	2.1	129
56	Scaling down the Perdew-Zunger self-interaction correction in many-electron regions. Journal of Chemical Physics, 2006, 124, 094108.	3.1	126
57	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.	7.6	122
58	DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. Physical Chemistry Chemical Physics, 2022, 24, 28700-28781.	2.9	122
59	What do the Kohn-Sham Orbital Energies Mean? How do Atoms Dissociate?. , 1985, , 265-308.		111
60	Rehabilitation of the Perdew-Burke-Ernzerhof generalized gradient approximation for layered materials. Physical Review B, 2017, 95, .	3.3	106
61	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. Physical Review A, 2008, 77, .	2.5	105
62	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	101
63	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	97
64	Relevance of the Slowly Varying Electron Gas to Atoms, Molecules, and Solids. Physical Review Letters, 2006, 97, 223002.	8.0	94
65	Global Hybrid Functionals: A Look at the Engine under the Hood. Journal of Chemical Theory and Computation, 2010, 6, 3688-3703.	5.6	90
66	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. Journal of Chemical Physics, 2021, 154, 061101.	3.1	89
67	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, .	3.3	87
68	Gedanken densities and exact constraints in density functional theory. Journal of Chemical Physics, 2014, 140, 18A533.	3.1	84
69	Density-gradient analysis for density functional theory: Application to atoms. International Journal of Quantum Chemistry, 1997, 61, 835-845.	2.1	81
70	Full self-consistency in the Fermi-orbital self-interaction correction. Physical Review A, 2017, 95, .	2.5	81
71	Cobalt Intercalated Layered NiFe Double Hydroxides for the Oxygen Evolution Reaction. Journal of Physical Chemistry B, 2018, 122, 847-854.	2.7	81
72	Pair distribution function of the spin-polarized electron gas:â€ƒA first-principles analytic model for all uniform densities. Physical Review B, 2002, 66, .	3.3	77

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73	The RPA Atomization Energy Puzzle. Journal of Chemical Theory and Computation, 2010, 6, 127-134.	5.6	77
74	Bending Two-Dimensional Materials To Control Charge Localization and Fermi-Level Shift. Nano Letters, 2016, 16, 2444-2449.	9.5	75
75	Short-range correlation in the uniform electron gas: Extended Overhauser model. Physical Review B, 2001, 64, .	3.3	73
76	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 355-363.	5.6	71
77	Climbing the ladder of density functional approximations. MRS Bulletin, 2013, 38, 743-750.	4.2	71
78	High-Level Correlated Approach to the Jellium Surface Energy, without Uniform-Gas Input. Physical Review Letters, 2008, 100, 036401.	8.0	69
79	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. Physical Review B, 2011, 83, .	3.3	68
80	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.	7.6	68
81	Lattice constants from semilocal density functionals with zero-point phonon correction. Physical Review B, 2012, 85, .	3.3	66
82	Semilocal density functionals and constraint satisfaction. International Journal of Quantum Chemistry, 2016, 116, 847-851.	2.1	66
83	Long-range van der Waals attraction and alkali-metal lattice constants. Physical Review B, 2010, 81, .	3.3	65
84	Energies of organic molecules and atoms in density functional theory. International Journal of Quantum Chemistry, 2005, 101, 506-511.	2.1	64
85	Improved Description of Stereoelectronic Effects in Hydrocarbons Using Semilocal Density Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 888-891.	5.6	63
86	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. Journal of Chemical Physics, 2019, 151, 214108.	3.1	63
87	Nonempirical Construction of Current-Density Functionals from Conventional Density-Functional Approximations. Physical Review Letters, 2005, 95, 196403.	8.0	62
88	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, .	7.6	61
89	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.	7.6	60
90	Exchange-correlation hole of a generalized gradient approximation for solids and surfaces. Physical Review B, 2009, 79, .	3.3	59

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91	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.	2.6	58
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.	9.5	58
93	Local and Gradient-Corrected Density Functionals. ACS Symposium Series, 1996, , 453-462.	0.0	57
94	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	55
95	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.	7.6	53
96	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. Nature Communications, 2021, 12, 6359.	13.2	53
97	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. Physical Review A, 2008, 77, .	2.5	52
98	Longâ€range asymptotic behavior of groundâ€state wave functions, oneâ€matrices, and pair densities. Journal of Chemical Physics, 1996, 105, 2798-2803.	3.1	51
99	Response to Comment on â€œDensity functional theory is straying from the path toward the exact functionalâ€• Science, 2017, 356, 496-496.	20.9	51
100	Synergy of van der Waals and self-interaction corrections in transition metal monoxides. Physical Review B, 2017, 96, .	3.3	51
101	Origin of the size-dependence of the equilibrium van der Waals binding between nanostructures. Journal of Chemical Physics, 2018, 148, 074110.	3.1	49
102	Correlation entropy of the H2 molecule. International Journal of Quantum Chemistry, 1997, 61, 935-941.	2.1	48
103	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	3.1	48
104	Two avenues to self-interaction correction within Kohnâ€”Sham theory: unitary invariance is the shortcut. Molecular Physics, 2003, 101, 1363-1368.	1.7	46
105	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.	2.7	46
106	Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors. Physical Review B, 2019, 100, .	3.3	45
107	Fourteen easy lessons in density functional theory. International Journal of Quantum Chemistry, 2010, 110, 2801-2807.	2.1	42
108	Communication: Ionization potentials in the limit of large atomic number. Journal of Chemical Physics, 2010, 133, 241103.	3.1	41

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109	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	40
110	Interplay between test sets and statistical procedures in ranking DFT methods: The case of electron density studies. Mendeleev Communications, 2018, 28, 225-235.	1.7	40
111	Water Oxidation Catalyzed by Cobalt Oxide Supported on the Mattagamite Phase of CoTe₂. ACS Catalysis, 2016, 6, 7393-7397.	11.7	39
112	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. Physical Review A, 2007, 76, .	2.5	37
113	Perdew-Zunger self-interaction correction: How wrong for uniform densities and large-Z atoms?. Journal of Chemical Physics, 2019, 150, 174106.	3.1	37
114	Energies of isoelectronic atomic ions from a successful metageneralized gradient approximation and other density functionals. Physical Review A, 2004, 70, .	2.5	34
115	Real-space analysis of the exchange-correlation energy. International Journal of Quantum Chemistry, 1995, 56, 199-210.	2.1	33
116	Role of the exchange-correlation energy: Nature's glue. International Journal of Quantum Chemistry, 2000, 77, 814-818.	2.1	33
117	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	32
118	Paradox of Self-Interaction Correction. Advances in Atomic, Molecular and Optical Physics, 2015, , 1-14.	4.5	32
119	Workhorse minimally empirical dispersion-corrected density functional with tests for weakly bound systems: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mrow><mml:mi mathvariant="normal">r</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msup><mml:mi>SCAN</mml:mi><mml:mo>+</mml:mo> Physical Review B, 2022, 106, .	3.3	32
120	Uniform electron gas from the Colle-Salvetti functional: Missing long-range correlations. Physical Review A, 2001, 63, .	2.5	31
121	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.	3.1	30
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.	7.6	30
123	Construction of meta-GGA functionals through restoration of exact constraint adherence to regularized SCAN functionals. Journal of Chemical Physics, 2022, 156, 034109.	3.1	30
124	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	28
125	Spin resolution of the electron-gas correlation energy:â€ƒPositive same spin contributions. Physical Review B, 2004, 69, .	3.3	27
126	Properties of the exchange hole under an appropriate coordinate transformation. Journal of Chemical Physics, 2003, 119, 6457-6464.	3.1	26

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127	Nonempirical density functionals investigated for jellium: Spin-polarized surfaces, spherical clusters, and bulk linear response. Physical Review B, 2008, 77, .	3.3	26
128	Structural phase transitions in Si and 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>crystals via the random phase approximation. Physical Review B, 2012, 86, .	3.3	26
129	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. Physical Review Letters, 2016, 117, 133002.	8.0	26
130	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.	3.1	25
131	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	24
132	Communication: Non-additivity of van der Waals interactions between nanostructures. Journal of Chemical Physics, 2014, 141, 141101.	3.1	24
133	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.	5.6	24
134	Accurate Density Functional for the Energy: Real-Space Cutoff of the Gradient Expansion for the Exchange Hole. Physical Review Letters, 1985, 55, 2370-2370.	8.0	23
135	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
136	Energetics of small clusters of stabilized jellium: Continuum and shell-structure effects. International Journal of Quantum Chemistry, 1993, 48, 249-261.	2.1	22
137	Simple physical picture of the Overhauser screened electron-electron interaction. Physical Review B, 2004, 69, .	3.3	22
138	Anisotropic Conductivity at the Singleâ€Molecule Scale. Angewandte Chemie - International Edition, 2019, 58, 14275-14280.	14.8	22
139	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. Journal of Chemical Physics, 2016, 144, 191101.	3.1	21
140	Simple charge-transfer model to explain the electrical response of hydrogen chains. Physical Review A, 2008, 78, .	2.5	20
141	Constraint-based wave vector and frequency dependent exchange-correlation kernel of the uniform electron gas. Physical Review B, 2020, 101, .	3.3	20
142	Screened van der Waals correction to density functional theory for solids. Physical Review Materials, 2017, 1, .	2.5	20
143	van der Waals Correction to the Physisorption of Graphene on Metal Surfaces. Journal of Physical Chemistry C, 2019, 123, 13748-13757.	3.3	19
144	Comment on â€œFunctional derivative of the universal density functional in Fock spaceâ€• Physical Review A, 2009, 79, .	2.5	17

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145	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. Molecular Physics, 2009, 107, 1077-1088.	1.7	17
146	Self-interaction correction in waterâ€“ion clusters. Journal of Chemical Physics, 2021, 154, 094302.	3.1	17
147	How accurate are the parametrized correlation energies of the uniform electron gas?. Physical Review B, 2018, 97, .	3.3	16
148	Density-functional energy gaps of solids demystified. European Physical Journal B, 2018, 91, 1.	1.6	16
149	van der Waals interaction as a summable asymptotic series. Physical Review A, 2012, 86, .	2.5	15
150	LONG-RANGE VAN DER WAALS INTERACTION. International Journal of Modern Physics B, 2013, 27, 1330011.	1.9	15
151	Modeling the physisorption of graphene on metals. Physical Review B, 2018, 97, .	3.3	15
152	Symmetry Breaking with the SCAN Density Functional Describes Strong Correlation in the Singlet Carbon Dimer. Journal of Physical Chemistry A, 2023, 127, 384-389.	2.6	15
153	First-principles study of the binding energy between nanostructures and its scaling with system size. Physical Review B, 2018, 97, .	3.3	13
154	Simple self-interaction correction to random-phase-approximation-like correlation energies. Physical Review A, 2019, 100, .	2.5	13
155	Understanding Density-Driven Errors for Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2023, 19, 532-543.	5.6	13
156	Infrared Properties of Molecular Cirrus. II. Cloudâ€toâ€Cloud Variations in Graphite and Polycyclic Aromatic Hydrocarbon Content. Astrophysical Journal, 2000, 536, 831-844.	4.7	12
157	EXPLORING THE ADIABATIC CONNECTION BETWEEN WEAK- AND STRONG-INTERACTION LIMITS IN DENSITY FUNCTIONAL THEORY. International Journal of Modern Physics B, 2001, 15, 1672-1683.	1.9	12
158	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. Journal of Physics Condensed Matter, 2012, 24, 424207.	1.9	12
159	Collapse of the electron gas from three to two dimensions in Kohn-Sham density functional theory. Physical Review B, 2018, 98, .	3.3	12
160	Exploring and enhancing the accuracy of interior-scaled Perdewâ€“Zunger self-interaction correction. Journal of Chemical Physics, 2021, 154, 094105.	3.1	12
161	Laplacian-level meta-generalized gradient approximation for solid and liquid metals. Physical Review Materials, 2022, 6, .	2.5	12
162	How metals bind: The deformable-jellium model with correlated electrons. American Journal of Physics, 2003, 71, 1048-1061.	0.8	11

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163	Predictive design of intrinsic half-metallicity in zigzag tungsten dichalcogenide nanoribbons. Physical Review B, 2019, 100, .	3.3	10
164	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.	3.1	10
165	Artificial intelligence â€œseesâ€•split electrons. Science, 2021, 374, 1322-1323.	20.9	10
166	First-principles wave-vector- and frequency-dependent exchange-correlation kernel for jellium at all densities. Physical Review B, 2022, 105, .	3.3	9
167	Van der Waals coefficients beyond the classical shell model. Journal of Chemical Physics, 2015, 142, 024312.	3.1	8
168	Density functionals combined with van der Waals corrections for graphene adsorbed on layered materials. Physical Review B, 2020, 101, .	3.3	8
169	Density-related properties from self-interaction corrected density functional theory calculations. Journal of Chemical Physics, 2021, 154, 024102.	3.1	8
170	Different bonding type along each crystallographic axis: Computational study of poly(p -phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.5	8
171	The two pillars: density and spin-density functional theories. Molecular Physics, 2016, 114, 928-931.	1.7	7
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.	22.2	7
173	DENSITY FUNCTIONALS AND SMALL INTERPARTICLE SEPARATIONS IN ELECTRONIC SYSTEMS. Modern Physics Letters B, 1995, 09, 829-838.	1.9	6
174	Anisotropic Conductivity at the Singleâ€Molecule Scale. Angewandte Chemie, 2019, 131, 14413-14418.	2.1	6
175	Calculation and interpretation of classical turning surfaces in solids. Npj Computational Materials, 2021, 7, .	9.1	6
176	Uniform Density Limit of Exchange-Correlation Energy Functionals. ACS Symposium Series, 2007, , 13-25.	0.0	5
177	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.	3.1	5
178	Initial Fermi orbital descriptors for FLOSIC calculations: The quick-FOD method. Chemical Physics Letters, 2021, 780, 138952.	2.7	4
179	Fermiâ€“LÃ¶wdin orbital self-interaction correction of adsorption energies on transition metal ions. Journal of Chemical Physics, 2022, 156, 134102.	3.1	4
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