

Correlation-energy functional and its high-density limit coupling-constant perturbation expansion

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Citation Report

#	ARTICLE	IF	CITATIONS
1	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
2	Recent constrained-search advances for approximating density functionals. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1994, 69, 763-769.	0.6	30
3	Exact Kohn-Sham scheme based on perturbation theory. <i>Physical Review A</i> , 1994, 50, 196-204.	1.0	506
4	New approach in the microscopic Fermi systems theory. <i>Physics Reports</i> , 1994, 249, 1-134.	10.3	148
5	Density functionals for the Yukawa electron-electron interaction. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 327-332.	1.0	261
6	DFT ionization formulas and aDFT perturbation theory for exchange and correlation, through adiabatic connection. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 93-108.	1.0	142
7	Energy differences between Kohn-Sham and Hartree-Fock wave functions yielding the same electron density. <i>Physical Review A</i> , 1995, 51, 4501-4513.	1.0	126
8	Bounds for the exchange and correlation potentials. <i>Physical Review A</i> , 1995, 51, 2851-2856.	1.0	15
9	Hardness of molecules and the band gap of solids within the Kohn-Sham formalism: A perturbation-scaling approach. <i>Physical Review A</i> , 1995, 52, 4493-4499.	1.0	74
10	Coordinate Scaling Requirements for Approximating Exchange and Correlation. <i>NATO ASI Series Series B: Physics</i> , 1995, , 11-31.	0.2	10
11	Generalized Kohn-Sham schemes and the band-gap problem. <i>Physical Review B</i> , 1996, 53, 3764-3774.	1.1	1,075
12	Elementary Concepts in Density Functional Theory. <i>Theoretical and Computational Chemistry</i> , 1996, , 3-24.	0.2	12
13	Density-functional theory for excited states. <i>Physical Review A</i> , 1996, 54, 3912-3915.	1.0	335
14	Expansions of the correlation-energy density functional $E_c[\rho]$ and its kinetic-energy component $T_c[\rho]$ in terms of homogeneous functionals. <i>Physical Review A</i> , 1996, 53, 2211-2219.	1.0	108
15	Expansions of the pair distribution function and the second-order density matrix in terms of homogeneous functionals. <i>Physical Review A</i> , 1996, 54, 4863-4867.	1.0	19
16	Simple modification of the Lee-Yang-Parr correlation functional to satisfy exact nonuniform scaling requirements. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1403-1407.	1.0	0
17	Applications to atoms, ions, and molecules of a novel form of the correlation energy density functional. <i>Chemical Physics Letters</i> , 1996, 257, 68-74.	1.2	17
18	Construction of the adiabatic connection. <i>Chemical Physics Letters</i> , 1996, 263, 499-506.	1.2	164

#	ARTICLE	IF	CITATIONS
19	Refinement of the Asymptotic Z Expansion for the Ground-State Correlation Energies of Atomic Ions. The Journal of Physical Chemistry, 1996, 100, 6167-6172.	2.9	110
20	Approach to density-functional ionization energy. Physical Review B, 1996, 53, 969-972.	1.1	10
21	Density-functional exchange identity from coordinate scaling. Physical Review A, 1996, 53, 3140-3142.	1.0	42
22	Coordinate scaling and adiabatic-connection formulation in density-functional theory. Physical Review A, 1997, 56, 1646-1649.	1.0	11
23	Hybrid schemes combining the Hartree-Fock method and density-functional theory: Underlying formalism and properties of correlation functionals. Journal of Chemical Physics, 1997, 106, 2675-2680.	1.2	97
24	Density functional theory and density matrices. , 1996, , 327-345.		1
25	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
26	Coupling-constant dependence of atomization energies. International Journal of Quantum Chemistry, 1997, 64, 285-295.	1.0	174
28	The adiabatic connection method: a non-empirical hybrid. Chemical Physics Letters, 1997, 265, 115-120.	1.2	212
29	Laurent series expansions in density functional theory. Chemical Physics Letters, 1997, 267, 14-22.	1.2	18
30	Padé approximants in density functional theory. Chemical Physics Letters, 1997, 268, 76-85.	1.2	12
31	Padé approximation for the polynomial representation of the correlation energy density functional. Chemical Physics Letters, 1997, 270, 443-452.	1.2	13
32	Toward reliable adiabatic connection models free from adjustable parameters. Chemical Physics Letters, 1997, 274, 242-250.	1.2	706
33	A numerical study of the functional derivative of the kinetic part of the density functional correlation energy. Chemical Physics Letters, 1998, 288, 338-342.	1.2	8
34	Hybrid methods: Combining density functional and wavefunction theory. , 1998, , 60-90.		5
35	Structure of the Pauli and Correlation-Kinetic Components of the Kohn-Sham Exchange Potential at a Metal Surface. Annals of Physics, 1998, 268, 149-171.	1.0	7
36	Optimized potential method for ensembles of excited states. International Journal of Quantum Chemistry, 1998, 69, 247-254.	1.0	34
37	Exact exchange kernel for time-dependent density-functional theory. International Journal of Quantum Chemistry, 1998, 69, 265-277.	1.0	81

#	ARTICLE	IF	CITATIONS
38	Generation of explicit electron correlation functional by means of local scaling transformations. International Journal of Quantum Chemistry, 1998, 69, 439-450.	1.0	6
39	Exact modified-Hartree-Fock scheme through perturbation expansion of density matrices. International Journal of Quantum Chemistry, 1998, 69, 469-483.	1.0	1
40	Polynomial and Padé ^{1/2} Representations for the Kinetic Component T_c of the Correlation Energy Density Functional. International Journal of Quantum Chemistry, 1998, 69, 513-522.	1.0	10
41	A new Wigner-like correlation-energy functional from coordinate scaling requirements. International Journal of Quantum Chemistry, 1998, 69, 523-532.	1.0	7
42	Virial exchange-correlation energy density in Hooke's atom. International Journal of Quantum Chemistry, 1998, 69, 533-540.	1.0	16
43	Density functional theory in relation to x-ray and neutron scattering experiments. International Journal of Quantum Chemistry, 1998, 69, 551-557.	1.0	1
44	Excited states in density functional theory. International Journal of Quantum Chemistry, 1998, 70, 681-691.	1.0	63
45	Density functionals for non-relativistic coulomb systems. , 1998, , 8-59.		22
46	Closed-form expression relating the second-order component of the density functional theory correlation energy to its functional derivative. Journal of Chemical Physics, 1998, 109, 6280-6286.	1.2	8
47	Connections between High-Density Scaling Limits of DFT Correlation Energies and Second-Order Z^{-1} Quantum Chemistry Correlation Energy. Journal of Physical Chemistry A, 1998, 102, 3151-3156.	1.1	20
48	Intermolecular Proton Transfer between Two Methylamine Molecules with an External Electric Field in the Gas Phase. Journal of Physical Chemistry A, 1998, 102, 7181-7190.	1.1	24
49	Nonlocality of the density functional for exchange and correlation: Physical origins and chemical consequences. Journal of Chemical Physics, 1998, 108, 1522-1531.	1.2	88
50	Exchange and correlation in silicon. Physical Review B, 1998, 57, 8972-8982.	1.1	117
51	Coupling-constant dependence of the density functional correlation energy. Journal of Chemical Physics, 1998, 109, 5212-5220.	1.2	22
52	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
53	Unambiguous exchange-correlation energy density. Journal of Chemical Physics, 1998, 109, 8161-8167.	1.2	109
54	Digging into the Exchange-Correlation Energy: The Exchange-Correlation Hole. , 1998, , 19-29.		2
55	Second-Order Relations Involving Correlation Energy and its Functional Derivative. Advances in Quantum Chemistry, 1998, 33, 11-29.	0.4	3

#	ARTICLE	IF	CITATIONS
56	ELECTRON DENSITY FUNCTIONAL THEORY. International Journal of Modern Physics B, 1999, 13, 511-523.	1.0	4
57	Connections between the correlation potential and the static correlation kernel for two-electron densities in high-density limit. Chemical Physics Letters, 1999, 308, 449-455.	1.2	9
58	Electron correlations in Kohn-Sham exchange-only theory. International Journal of Quantum Chemistry, 1999, 71, 473-480.	1.0	7
59	Correlation energy contributions from low-lying states to density functionals based on an electron gas with a gap. International Journal of Quantum Chemistry, 1999, 75, 885-888.	1.0	20
60	A fresh look at ensembles: Derivative discontinuities in density functional theory. Journal of Chemical Physics, 1999, 110, 4710-4723.	1.2	73
61	Comparison of Hartree-Fock and Kohn-Sham determinants as wave functions. Journal of Computational Chemistry, 2000, 21, 8-16.	1.5	17
62	Bounding the extrapolated correlation energy using Padé _{1/2} approximants. International Journal of Quantum Chemistry, 2000, 79, 222-234.	1.0	13
63	Excitation energies from time-dependent density functional theory using exact and approximate potentials. International Journal of Quantum Chemistry, 2000, 80, 534-554.	1.0	57
64	Analytical properties of the Kohn-Sham theory exchange and correlation energy and potential via quantal density functional theory. International Journal of Quantum Chemistry, 2000, 80, 555-566.	1.0	31
65	Application of the scaling properties of the correlation energy functional to local and gradient-dependent forms. Chemical Physics Letters, 2000, 322, 371-376.	1.2	0
66	Adiabatic perturbation theory for Van der Waals coefficients. Computational and Theoretical Chemistry, 2000, 501-502, 271-276.	1.5	4
67	An exact second-order expression for the density functional theory correlation potential for molecules. Journal of Chemical Physics, 2001, 114, 1952-1955.	1.2	23
68	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
69	An alternative optimized potential method for ensembles of excited states. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 2363-2370.	0.6	29
70	Sum rules for exchange and correlation potentials. Journal of Chemical Physics, 2001, 115, 4438-4443.	1.2	39
71	Second-order truncated functional expansions of energy density functionals. Physical Review A, 2001, 64, .	1.0	3
72	Effective action and density-functional theory. Physical Review B, 2002, 66, .	1.1	39
73	Finite-basis-set optimized effective potential exchange-only method. Journal of Chemical Physics, 2002, 116, 1269-1276.	1.2	62

#	ARTICLE	IF	CITATIONS
74	Accurate correlation potentials from integral formulation of density functional perturbation theory. <i>Journal of Chemical Physics</i> , 2002, 116, 6924-6929.	1.2	24
75	Optimized Effective Potential Method and KLI Approximation for Systems with Degenerate Orbitals in the LCAO Calculations. <i>Journal of the Physical Society of Japan</i> , 2002, 71, 470-475.	0.7	0
76	Ab-initio density functional theory: OEP-MBPT(2). A new orbital-dependent correlation functional. <i>Journal of Chemical Physics</i> , 2002, 116, 4415-4425.	1.2	139
77	Density functional theory from the extreme limits of correlation. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 145-150.	1.0	8
78	Study of subspace density functional theory application of LSDA to excited states of atoms. <i>International Journal of Quantum Chemistry</i> , 2003, 92, 234-238.	1.0	6
79	Adiabatic connection approach to density functional theory of electronic systems. <i>International Journal of Quantum Chemistry</i> , 2003, 93, 166-190.	1.0	87
80	Development and implementation of the exact exchange method for semiconductors using a localized basis set. <i>Computational Materials Science</i> , 2003, 28, 274-286.	1.4	22
81	Density Functionals for Non-relativistic Coulomb Systems in the New Century. <i>Lecture Notes in Physics</i> , 2003, , 1-55.	0.3	96
82	Advantages and limitations of Kohn-Sham orbitals as single electron basis for multireference configuration interaction and multireference perturbation theory. <i>Journal of Chemical Physics</i> , 2003, 119, 11591-11601.	1.2	27
83	Connections between second-order Green's function-Levy and many-body perturbation approaches in density functional theory. <i>Journal of Chemical Physics</i> , 2003, 118, 461-470.	1.2	28
84	Integral expressions satisfied by the gradient of density functional potentials. <i>Journal of Chemical Physics</i> , 2003, 119, 1916-1921.	1.2	3
85	Asymptotic behavior of the exchange-correlation potentials from the linear-response Sham-Schlüter equation. <i>Journal of Chemical Physics</i> , 2003, 118, 9504-9518.	1.2	47
86	Theories for excited states. <i>Advances in Quantum Chemistry</i> , 2003, 42, 363-381.	0.4	11
87	Formally Exact Exchange-Correlation Potential in a Local-Scaling Density Functional Theory. <i>Journal of the Physical Society of Japan</i> , 2003, 72, 1926-1931.	0.7	4
88	Double excitations within time-dependent density functional theory linear response. <i>Journal of Chemical Physics</i> , 2004, 120, 5932-5937.	1.2	431
89	Potential-energy surfaces for excited states in extended systems. <i>Journal of Chemical Physics</i> , 2004, 120, 4593-4602.	1.2	103
90	Adiabatic connection for near degenerate excited states. <i>Physical Review A</i> , 2004, 69, .	1.0	26
91	Density-functional theory in one dimension for contact-interacting fermions. <i>Physical Review A</i> , 2004, 70, .	1.0	55

#	ARTICLE	IF	CITATIONS
92	Exact analytic total energy functional for Hooke's atom generated by local-scaling transformations. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 297-307.	1.0	18
93	Theories for individual excited states. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 256-264.	1.0	7
94	A dressed TDDFT treatment of the 21Ag states of butadiene and hexatriene. <i>Chemical Physics Letters</i> , 2004, 389, 39-42.	1.2	192
95	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. <i>Journal of Chemical Physics</i> , 2004, 120, 6898-6911.	1.2	431
96	Intermolecular potential energy surfaces of weakly bound dimers computed from ab initio density functional theory: The right answer for the right reason. <i>Chemical Physics Letters</i> , 2005, 405, 43-48.	1.2	62
97	First-order correlation-kinetic contribution to Kohn-Sham exchange charge density function in atoms, using quantum density functional theory approach. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 231-238.	1.0	4
98	Avoiding asymptotic divergence of the potential from orbital- and energy-dependent exchange-correlation functionals. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 635-644.	1.0	19
99	Novel properties of the Kohn-Sham exchange potential for open systems: Application to the two-dimensional electron gas. <i>Europhysics Letters</i> , 2005, 70, 116-122.	0.7	11
100	Orbital-dependent correlation energy in density-functional theory based on a second-order perturbation approach: Success and failure. <i>Journal of Chemical Physics</i> , 2005, 123, 062204.	1.2	99
101	Ab initio density functional theory: The best of both worlds?. <i>Journal of Chemical Physics</i> , 2005, 123, 062205.	1.2	160
102	Exact and approximate exchange potentials investigated in terms of their matrix elements with the Kohn-Sham orbitals. <i>Physical Review A</i> , 2005, 72, .	1.0	20
103	Generalized density functional theory for degenerate states. <i>Journal of Chemical Physics</i> , 2005, 122, 134107.	1.2	28
104	Relations between coordinate and potential scaling in the high-density limit. <i>Journal of Chemical Physics</i> , 2005, 122, 134108.	1.2	6
105	Combining GW calculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. <i>New Journal of Physics</i> , 2005, 7, 126-126.	1.2	263
106	Describing static correlation in bond dissociation by Kohn-Sham density functional theory. <i>Journal of Chemical Physics</i> , 2005, 122, 094116.	1.2	183
107	Fluctuation-dissipation theorem density-functional theory. <i>Journal of Chemical Physics</i> , 2005, 122, 164106.	1.2	196
108	Density scaling and exchange-correlation energy. <i>Journal of Chemical Physics</i> , 2005, 123, 044105.	1.2	15
109	Towards chemical accuracy for the thermodynamics of large molecules: new hybrid density functionals including non-local correlation effects. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4398.	1.3	538

#	ARTICLE	IF	CITATIONS
110	Calculating state-to-state transition probabilities within time-dependent density-functional theory. <i>Physical Review A</i> , 2006, 74, .	1.0	27
111	Self-interaction-free exchange-correlation functional for thermochemistry and kinetics. <i>Journal of Chemical Physics</i> , 2006, 124, 091102.	1.2	179
112	Scaling relations, virial theorem, and energy densities for long-range and short-range density functionals. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2026-2034.	1.0	21
113	Double-pole approximation in time-dependent density functional theory. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2840-2847.	1.0	6
114	Ab initio DFT: Getting the right answer for the right reason. <i>Computational and Theoretical Chemistry</i> , 2006, 771, 1-8.	1.5	49
115	The method of increments—a wavefunction-based ab initio correlation method for solids. <i>Physics Reports</i> , 2006, 428, 1-52.	10.3	209
116	Ab initio correlation functionals from second-order perturbation theory. <i>Journal of Chemical Physics</i> , 2006, 125, 104108.	1.2	58
117	Optimized effective potential from a correlated wave function: Optimized effective potential-generalized valence bond (OEP-GVB). <i>Journal of Chemical Physics</i> , 2006, 125, 054101.	1.2	11
118	Exchange-correlation energy in molecules: A variational quantum Monte Carlo study. <i>Physical Review A</i> , 2006, 74, .	1.0	9
119	Optimized effective potential in real time: Problems and prospects in time-dependent density-functional theory. <i>Physical Review A</i> , 2006, 74, .	1.0	30
120	Localized exchange-correlation potential from second-order self-energy for accurate Kohn-Sham energy gap. <i>Journal of Chemical Physics</i> , 2007, 126, 214102.	1.2	31
121	Modeling the adiabatic connection in H ₂ . <i>Journal of Chemical Physics</i> , 2007, 126, 244104.	1.2	34
122	Assessment and formal properties of exchange-correlation functionals constructed from the adiabatic connection. <i>Journal of Chemical Physics</i> , 2007, 127, 034101.	1.2	59
123	Noniterative accurate algorithm for the exact exchange potential of density-functional theory. <i>Physical Review A</i> , 2007, 76, .	1.0	7
124	Alternative derivation of an exchange-only density-functional optimized effective potential. <i>Physical Review A</i> , 2007, 76, .	1.0	3
125	Signatures of Discontinuity in the Exchange-Correlation Energy Functional Derived from the Subband Electronic Structure of Semiconductor Quantum Wells. <i>Physical Review Letters</i> , 2007, 98, 066806.	2.9	20
126	Exchange and correlation near the nucleus in density functional theory. <i>Physical Review B</i> , 2007, 75, .	1.1	18
127	Asymptotic form of the Kohn-Sham correlation potential. <i>Physical Review A</i> , 2007, 76, .	1.0	6

#	ARTICLE	IF	CITATIONS
128	Meta-generalized gradient approximation: non-empirical construction and performance of a density functional. <i>Philosophical Magazine</i> , 2007, 87, 1071-1084.	0.7	11
129	Analytic derivatives for perturbatively corrected "double hybrid" density functionals: Theory, implementation, and applications. <i>Journal of Chemical Physics</i> , 2007, 126, 124115.	1.2	173
130	Double-hybrid density functionals with long-range dispersion corrections: higher accuracy and extended applicability. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 3397.	1.3	979
131	Adiabatic connection in density-functional theory: Two electrons on the surface of a sphere. <i>Physical Review A</i> , 2007, 75, .	1.0	36
132	Highly Accurate First-Principles Benchmark Data Sets for the Parametrization and Validation of Density Functional and Other Approximate Methods. Derivation of a Robust, Generally Applicable, Double-Hybrid Functional for Thermochemistry and Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12868-12886.	1.1	680
133	Double-Hybrid Functionals for Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3-8.	1.1	213
134	Developing the random phase approximation into a practical post-Kohn-Sham correlation model. <i>Journal of Chemical Physics</i> , 2008, 129, 114105.	1.2	246
135	Self-consistent many-body perturbation theory in range-separated density-functional theory: A one-electron reduced-density-matrix-based formulation. <i>Physical Review A</i> , 2008, 78, .	1.0	56
136	A Systematic Density Functional Study of the Zero-Field Splitting in Mn(II) Coordination Compounds. <i>Inorganic Chemistry</i> , 2008, 47, 134-142.	1.9	121
137	Semiempirical Double-Hybrid Density Functional with Improved Description of Long-Range Correlation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2702-2712.	1.1	123
138	Theoretical Thermodynamics for Large Molecules: Walking the Thin Line between Accuracy and Computational Cost. <i>Accounts of Chemical Research</i> , 2008, 41, 569-579.	7.6	329
139	Embedding a multideterminantal wave function in an orbital-free environment. <i>Physical Review A</i> , 2008, 77, .	1.0	138
140	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. <i>Physical Review A</i> , 2008, 78, .	1.0	221
141	What can we learn from the adiabatic connection formalism about local hybrid functionals?. <i>Journal of Chemical Physics</i> , 2008, 128, 214107.	1.2	44
142	Adiabatic connection forms in density functional theory: H ₂ and the He isoelectronic series. <i>Journal of Chemical Physics</i> , 2008, 129, 064105.	1.2	21
143	Effect of the nonlocal exchange on the performance of the orbital-dependent correlation functionals from second-order perturbation theory. <i>Journal of Chemical Physics</i> , 2008, 129, 124109.	1.2	17
145	An inversion technique for the calculation of embedding potentials. <i>Journal of Chemical Physics</i> , 2008, 129, 184104.	1.2	93
146	Entanglement and density-functional theory: Testing approximations on Hooke's atom. <i>Physical Review B</i> , 2008, 77, .	1.1	82

#	ARTICLE	IF	CITATIONS
147	Extended Hartree-Fock method based on pair density functional theory. <i>Physical Review B</i> , 2008, 77, .	1.1	21
148	Density-density functionals and effective potentials in many-body electronic structure calculations. <i>Physical Review B</i> , 2008, 77, .	1.1	12
149	Rayleigh-Schrödinger many-body perturbation theory for density functionals: A unified treatment of one- and two-electron perturbations. <i>Physical Review A</i> , 2008, 78, .	1.0	25
150	Chapter 6 Generalized Kohn-Sham Density Functional Theory via Effective Action Formalism. <i>Handbook of Metal Physics</i> , 2008, 4, 131-156.	0.0	1
151	Stretched hydrogen molecule from a constrained-search density-functional perspective. <i>Physical Review A</i> , 2009, 80, .	1.0	6
152	Adiabatic connection in the low-density limit. <i>Physical Review A</i> , 2009, 79, .	1.0	30
153	Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 4963-4968.	3.3	332
154	Chapter 4 Reflections on Formal Density Functional Theory. <i>Advances in Quantum Chemistry</i> , 2009, 56, 181-216.	0.4	3
155	Dependence of Response Functions and Orbital Functionals on Occupation Numbers. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 693-698.	2.3	3
156	Extension to Negative Values of the Coupling Constant of Adiabatic Connection for Interaction-Strength Interpolation. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 708-711.	2.3	13
157	The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems. <i>Journal of Chemical Physics</i> , 2009, 130, 104111.	1.2	64
158	Formal expressions and corresponding expansions for the exact Kohn-Sham exchange potential. <i>Physical Review A</i> , 2009, 80, .	1.0	10
159	Optimization and Basis-Set Dependence of a Restricted-Open-Shell Form of B2-PLYP Double-Hybrid Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9861-9873.	1.1	77
160	Out of one, many â€” Using moment expansions of the virial relation to deduce universal density functionals from a single system. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1540-1545.	0.6	6
161	When does static correlation scale to the high-density limit as exchange does?. <i>Computational and Theoretical Chemistry</i> , 2010, 943, 19-22.	1.5	8
162	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. <i>Journal of Chemical Physics</i> , 2010, 132, 194105.	1.2	40
163	Communication: Constrained search formulation of the ground state energy as a functional of an idempotent one-matrix. <i>Journal of Chemical Physics</i> , 2010, 133, 151102.	1.2	2
164	Basis set dependence of the doubly hybrid XYG3 functional. <i>Journal of Chemical Physics</i> , 2010, 133, 104105.	1.2	41

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165	Many-electron self-interaction and spin polarization errors in local hybrid density functionals. <i>Journal of Chemical Physics</i> , 2010, 133, 134116.	1.2	83
166	Range-dependent adiabatic connections. <i>Journal of Chemical Physics</i> , 2010, 133, 164112.	1.2	30
167	Accurate calculation and modeling of the adiabatic connection in density functional theory. <i>Journal of Chemical Physics</i> , 2010, 132, 164115.	1.2	86
168	Extending the reliability and applicability of B3LYP. <i>Chemical Communications</i> , 2010, 46, 3057.	2.2	196
169	Adiabatic connection at negative coupling strengths. <i>Physical Review A</i> , 2010, 81, .	1.0	13
170	Ab initio DFT – the seamless connection between WFT and DFT. <i>Molecular Physics</i> , 2010, 108, 3313-3322.	0.8	15
171	An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 727-734.	2.3	91
172	Trends in R ^X Bond Dissociation Energies (R = Me, Et, i-Pr, t-Bu, X = H, Me, Cl, OH). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1462-1469.	2.3	39
173	DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20801-20808.	1.5	329
174	Density Functional Theory of Electronic Structure: A Short Course for Mineralogists and Geophysicists. <i>Reviews in Mineralogy and Geochemistry</i> , 2010, 71, 1-18.	2.2	16
175	Single-particle and quasiparticle interpretation of Kohn-Sham and generalized Kohn-Sham eigenvalues for hybrid functionals. <i>Physical Review B</i> , 2010, 82, .	1.1	58
176	Frontiers in electronic structure theory. <i>Journal of Chemical Physics</i> , 2010, 132, 110902.	1.2	147
177	Fast computation of molecular random phase approximation correlation energies using resolution of the identity and imaginary frequency integration. <i>Journal of Chemical Physics</i> , 2010, 132, 234114.	1.2	228
178	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. <i>International Reviews in Physical Chemistry</i> , 2011, 30, 115-160.	0.9	116
179	Double-hybrid density-functional theory made rigorous. <i>Journal of Chemical Physics</i> , 2011, 134, 064113.	1.2	165
180	Beyond the Random-Phase Approximation for the Electron Correlation Energy: The Importance of Single Excitations. <i>Physical Review Letters</i> , 2011, 106, 153003.	2.9	193
181	DSD-PBEP86: in search of the best double-hybrid DFT with spin-component scaled MP2 and dispersion corrections. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20104.	1.3	409
182	Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionals – Evaluation with the Extended GMTKN30 Database for General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 291-309.	2.3	1,035

#	ARTICLE	IF	CITATIONS
183	Dispersion interactions in density-functional theory: An adiabatic-connection analysis. <i>Journal of Chemical Physics</i> , 2011, 135, 194109.	1.2	21
184	Comparing <i>ab initio</i> density-functional and wave function theories: The impact of correlation on the electronic density and the role of the correlation potential. <i>Journal of Chemical Physics</i> , 2011, 135, 114111.	1.2	39
185	Progress at the interface of wave-function and density-functional theories. <i>Physical Review A</i> , 2011, 83, .	1.0	17
186	Basis set convergence of explicitly correlated double-hybrid density functional theory calculations. <i>Journal of Chemical Physics</i> , 2011, 135, 144119.	1.2	29
187	Random-phase approximation correlation methods for molecules and solids. <i>Molecular Physics</i> , 2011, 109, 2473-2500.	0.8	146
188	Failure of the Weizsäcker kinetic energy functional for one-, two-, and three-electron distribution functions. <i>Journal of Mathematical Chemistry</i> , 2011, 49, 1810-1821.	0.7	26
189	A theoretical model for electron transfer in ion-atom collisions: Calculations for the collision of a proton with an argon atom. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011, 375, 3290-3295.	0.9	27
190	Magnetic Properties of Paddlewheels and Trinuclear Clusters with Exposed Metal Sites. <i>ChemPhysChem</i> , 2011, 12, 3307-3319.	1.0	27
191	Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. <i>Journal of Computational Chemistry</i> , 2011, 32, 1824-1838.	1.5	26
192	Communication: Rationale for a new class of double-hybrid approximations in density-functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 101102.	1.2	93
193	Equation satisfied by the energy-density functional for electron-electron mutual Coulomb repulsion. <i>Physical Review A</i> , 2011, 84, .	1.0	4
194	Exact exchange potential evaluated from occupied Kohn-Sham and Hartree-Fock solutions. <i>Physical Review A</i> , 2011, 83, .	1.0	2
195	A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 19896-19900.	3.3	143
196	A simple but fully nonlocal correction to the random phase approximation. <i>Journal of Chemical Physics</i> , 2011, 134, 114110.	1.2	33
197	Time-dependent density functional theory of open quantum systems in the linear-response regime. <i>Journal of Chemical Physics</i> , 2011, 134, 074116.	1.2	22
198	Assessment of correlation energies based on the random-phase approximation. <i>New Journal of Physics</i> , 2012, 14, 043002.	1.2	137
199	Non-empirical improvement of PBE and its hybrid PBE0 for general description of molecular properties. <i>Journal of Chemical Physics</i> , 2012, 136, 104108.	1.2	78
200	Comment on "Exact relation in the density functional theory" by Bobrov V. B. et al.. <i>Europhysics Letters</i> , 2012, 97, 17001.	0.7	3

#	ARTICLE	IF	CITATIONS
201	Reply to the Comment by D. P. Joubert. Europhysics Letters, 2012, 97, 17002.	0.7	0
202	B2-PPW91: A promising double-hybrid density functional for the electric response properties. Journal of Chemical Physics, 2012, 136, 124111.	1.2	30
203	Coupling-constant expression and exact relations for the kinetic-energy functional in pair-density-functional theory. Physical Review A, 2012, 85, .	1.0	7
204	Functional relations for the density-functional exchange and correlation functionals connecting functionals at three densities. Physical Review A, 2012, 85, .	1.0	1
205	Discontinuities of the exchange-correlation kernel and charge-transfer excitations in time-dependent density-functional theory. Physical Review A, 2012, 85, .	1.0	77
206	Constraint on the second functional derivative of the exchange-correlation energy. Molecular Physics, 2012, 110, 2275-2279.	0.8	0
207	Random-phase approximation and its applications in computational chemistry and materials science. Journal of Materials Science, 2012, 47, 7447-7471.	1.7	479
208	Accurate Spin-State Energetics of Transition Metal Complexes. 1. CCSD(T), CASPT2, and DFT Study of $[M(NCH_6)]^{2+}$ (M = Fe, Co). Journal of Chemical Theory and Computation, 2012, 8, 4216-4231.	2.3	130
209	Energy Densities in the Strong-Interaction Limit of Density Functional Theory. Journal of Chemical Theory and Computation, 2012, 8, 3097-3107.	2.3	43
210	Comparative Study of Single and Double Hybrid Density Functionals for the Prediction of 3d Transition Metal Thermochemistry. Journal of Chemical Theory and Computation, 2012, 8, 4102-4111.	2.3	69
211	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. Journal of Chemical Physics, 2012, 136, 174103.	1.2	99
212	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. Physical Chemistry Chemical Physics, 2012, 14, 12554.	1.3	32
213	Note: Theoretical mixing coefficients for hybrid functionals. Journal of Chemical Physics, 2012, 136, 086101.	1.2	36
214	Spin-component-scaled electron correlation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 886-906.	6.2	197
215	Challenges for Density Functional Theory. Chemical Reviews, 2012, 112, 289-320.	23.0	1,869
216	Gas-Phase Thermodynamics as a Validation of Computational Catalysis on Surfaces: A Case Study of Fischer-Tropsch Synthesis. ChemPhysChem, 2012, 13, 1486-1494.	1.0	23
217	Comparison of three methods for calculation of electron transfer probability in $H^{++}Ne$. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 469-471.	0.9	12
218	Electron correlation methods based on the random phase approximation. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	353

#	ARTICLE	IF	CITATIONS
219	Some formal properties of ensemble density functionals. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1076-1085.	1.0	2
220	Spin-component-scaled double hybrids: An extensive search for the best fifth-generation functionals blending DFT and perturbation theory. <i>Journal of Computational Chemistry</i> , 2013, 34, 2327-2344.	1.5	292
221	Theoretical investigation of the electron capture and loss processes in the collisions of He ²⁺ + Ne. <i>Journal of Chemical Physics</i> , 2013, 139, 084321.	1.2	7
222	Communication: Random phase approximation renormalized many-body perturbation theory. <i>Journal of Chemical Physics</i> , 2013, 139, 171103.	1.2	93
223	Influence of the exchange-correlation potential in methods based on time-dependent density-functional theory. <i>Physical Review A</i> , 2013, 88, .	1.0	15
224	Optimized effective potential method based on spin-resolved components of the second-order correlation energy in density functional theory. <i>Physical Review B</i> , 2013, 87, .	1.1	26
225	Analysis of double-hybrid density functionals along the adiabatic connection. <i>Molecular Physics</i> , 2013, 111, 1275-1294.	0.8	42
226	Validation of Double-Hybrid Density Functionals for Electric Response Properties of Transition-Metal Systems: A New Paradigm Based on Physical Considerations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2884-2890.	1.1	11
227	Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. <i>Journal of Computational Chemistry</i> , 2013, 34, 1759-1774.	1.5	26
228	A simple DFT-based diagnostic for nondynamical correlation. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	114
229	Electron Correlation in the Condensed Phase from a Resolution of Identity Approach Based on the Gaussian and Plane Waves Scheme. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2654-2671.	2.3	113
230	How Well Can Parametrized and Parameter-Free Double-Hybrid Approximations Predict Response Properties of Hydrogen-Bonded Systems? Dipole Polarizabilities of Water Nanoclusters as a Working Model. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4506-4513.	1.1	17
231	Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1669-1675.	2.1	63
232	A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0. <i>Journal of Chemical Physics</i> , 2013, 139, 174106.	1.2	32
233	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. <i>Physical Review B</i> , 2013, 88, .	1.1	113
234	Discontinuous functional for linear-response time-dependent density-functional theory: The exact-exchange kernel and approximate forms. <i>Physical Review A</i> , 2013, 88, .	1.0	24
235	Communication: Double-hybrid functionals from adiabatic-connection: The QIDH model. <i>Journal of Chemical Physics</i> , 2014, 141, 031101.	1.2	154
236	Orbital-dependent second-order scaled-opposite-spin correlation functionals in the optimized effective potential method. <i>Journal of Chemical Physics</i> , 2014, 141, 024113.	1.2	35

#	ARTICLE	IF	CITATIONS
237	Correlation energy within exact-exchange adiabatic connection fluctuation-dissipation theory: Systematic development and simple approximations. <i>Physical Review B</i> , 2014, 90, .	1.1	41
238	Constricted Variational Density Functional Theory Approach to the Description of Excited States. <i>Topics in Current Chemistry</i> , 2014, 368, 61-95.	4.0	6
239	Ions in solution: Density corrected density functional theory (DC-DFT). <i>Journal of Chemical Physics</i> , 2014, 140, 18A528.	1.2	87
240	Perspective: Fifty years of density-functional theory in chemical physics. <i>Journal of Chemical Physics</i> , 2014, 140, 18A301.	1.2	1,083
241	Construction of a parameter-free doubly hybrid density functional from adiabatic connection. <i>Journal of Chemical Physics</i> , 2014, 140, 18A512.	1.2	57
243	Double-hybrid density functionals. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 576-600.	6.2	292
244	Fractional Charge Behavior and Band Gap Predictions with the XYG3 Type of Doubly Hybrid Density Functionals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9201-9211.	1.1	45
245	Reduced-density-matrix-functional theory at finite temperature: Theoretical foundations. <i>Physical Review A</i> , 2015, 92, .	1.0	29
246	Response to "Comment on "Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0â€™" [J. Chem. Phys. 143, 187101 (2015)]. <i>Journal of Chemical Physics</i> , 2015, 143, 187102.	1.2	8
247	Communication: Kohn-Sham theory for excited states of Coulomb systems. <i>Journal of Chemical Physics</i> , 2015, 143, 191101.	1.2	33
248	Probing the structural and dynamical properties of liquid water with models including non-local electron correlation. <i>Journal of Chemical Physics</i> , 2015, 143, 054506.	1.2	89
249	Construction of exchange-correlation functionals through interpolation between the non-interacting and the strong-correlation limit. <i>Journal of Chemical Physics</i> , 2015, 143, 124103.	1.2	23
250	Global Hybrids from the Semiclassical Atom Theory Satisfying the Local Density Linear Response. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 122-131.	2.3	22
251	Excited states from range-separated density-functional perturbation theory. <i>Molecular Physics</i> , 2015, 113, 1740-1749.	0.8	12
252	The Hubbard dimer: a density functional case study of a many-body problem. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 393001.	0.7	83
253	NTChem: A high-performance software package for quantum molecular simulation. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 349-359.	1.0	55
254	Density scaling and virial theorem. <i>Molecular Physics</i> , 2015, 113, 1839-1842.	0.8	1
255	Designing a paradigm for parameter-free double-hybrid density functionals through the adiabatic connection path. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	26

#	ARTICLE	IF	CITATIONS
256	Calculating excitation energies by extrapolation along adiabatic connections. <i>Physical Review A</i> , 2015, 91, .	1.0	14
257	H + H ₂ quantum dynamics using potential energy surfaces based on the XYG3 type of doubly hybrid density functionals: Validation of the density functionals. <i>Journal of Chemical Physics</i> , 2015, 142, 084107.	1.2	11
258	Systematic Improvement of Density Functionals through Parameter-Free Hybridization Schemes. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3540-3545.	2.1	44
259	Toward the construction of parameter-free doubly hybrid density functionals. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 589-595.	1.0	22
260	Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution. <i>Computer Physics Communications</i> , 2015, 187, 120-129.	3.0	42
261	Accurate, Precise, and Efficient Theoretical Methods To Calculate Anion-π Interaction Energies in Model Structures. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 360-371.	2.3	26
262	Mathematical thoughts in DFT. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 802-804.	1.0	12
263	Comparison of one-parameter and linearly scaled one-parameter double-hybrid density functionals for noncovalent interactions. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1166-1172.	1.0	5
264	Wave-function inspired density functional applied to the H ₂ ⁺ challenge. <i>New Journal of Physics</i> , 2016, 18, 073026.	1.2	12
265	SCAN-based hybrid and double-hybrid density functionals from models without fitted parameters. <i>Journal of Chemical Physics</i> , 2016, 144, 044114.	1.2	126
266	Exchange-Correlation Functionals via Local Interpolation along the Adiabatic Connection. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2598-2610.	2.3	40
267	Global hybrid exchange energy functional with correct asymptotic behavior of the corresponding potential. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
268	Seeking for Spin-Opposite-Scaled Double-Hybrid Models Free of Fitted Parameters. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3726-3730.	1.1	28
269	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. <i>Chemical Communications</i> , 2016, 52, 13840-13860.	2.2	18
270	Accurate Kohn-Sham ionization potentials from scaled-opposite-spin second-order optimized effective potential methods. <i>Journal of Computational Chemistry</i> , 2016, 37, 2081-2090.	1.5	24
271	Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists. <i>Accounts of Chemical Research</i> , 2016, 49, 1503-1513.	7.6	103
272	Kinetic-energy-density dependent semilocal exchange-correlation functionals. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1641-1694.	1.0	78
273	The XYG3 type of doubly hybrid density functionals. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016, 6, 721-747.	6.2	52

#	ARTICLE	IF	CITATIONS
274	Quadratic integrand double-hybrid made spin-component-scaled. <i>Journal of Chemical Physics</i> , 2016, 144, 124104.	1.2	31
275	A comparative study of the ω BH-PBE0 and DSD-PBEPBE-D3BJ doubly hybrid density functionals. <i>Molecular Physics</i> , 2016, 114, 1207-1217.	0.8	10
276	Development of New Density Functional Approximations. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 155-182.	4.8	51
277	Interpolated energy densities, correlation indicators and lower bounds from approximations to the strong coupling limit of DFT. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6169-6183.	1.3	28
278	Low scaling random-phase approximation electron correlation method including exchange interactions using localised orbitals. <i>Journal of Chemical Physics</i> , 2017, 146, 174110.	1.2	10
279	DSD-PBEP86-NL and DOD-PBEP86-NL functionals for noncovalent interactions: Basis set effects and tentative applications to large noncovalent systems. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25417.	1.0	6
280	Random-Phase Approximation Methods. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 421-445.	4.8	127
281	Properties of Augmented Kohn-Sham Potential for Energy as Simple Sum of Orbital Energies. <i>Journal of Physical Chemistry A</i> , 2017, 121, 342-347.	1.1	3
282	A local Fock-exchange potential in Kohn-Sham equations. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 04LT01.	0.7	12
283	Wigner crystallization in transition metal dichalcogenides: A new approach to correlation energy. <i>Physical Review B</i> , 2017, 95, .	1.1	22
284	DFT-inspired methods for quantum thermodynamics. <i>Scientific Reports</i> , 2017, 7, 4655.	1.6	15
285	Time-Dependent Double-Hybrid Density Functionals with Spin-Component and Spin-Opposite Scaling. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4307-4323.	2.3	60
286	Charge transfer in time-dependent density functional theory. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 423001.	0.7	89
287	Advances in modeling hydrocarbon cracking kinetic predictions by quantum chemical theory: A review. <i>International Journal of Energy Research</i> , 2018, 42, 3164-3181.	2.2	11
288	Doubly hybrid density functionals that correctly describe both density and energy for atoms. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 2287-2292.	3.3	36
289	Signatures of van der Waals binding: A coupling-constant scaling analysis. <i>Physical Review B</i> , 2018, 97, .	1.1	17
290	Excitation energies from $G\ddot{A}$ rling-Levy perturbation theory along the range-separated adiabatic connection. <i>Molecular Physics</i> , 2018, 116, 1443-1451.	0.8	5
291	A general range-separated double-hybrid density-functional theory. <i>Journal of Chemical Physics</i> , 2018, 148, 164105.	1.2	33

#	ARTICLE	IF	CITATIONS
292	Does the exchangeâ€“correlation kernel f_{xc} have a very long-ranged dependence on the groundstate electron density?. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	1
293	Optimal power series expansions of the Kohnâ€“Sham potential. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	5
294	Communication: Strong-interaction limit of an adiabatic connection in Hartree-Fock theory. <i>Journal of Chemical Physics</i> , 2018, 149, 241101.	1.2	25
295	Approximate energy functionals for one-body reduced density matrix functional theory from many-body perturbation theory. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	6
296	Extent of Fock-exchange mixing for a hybrid van der Waals density functional?. <i>Journal of Chemical Physics</i> , 2018, 148, 194115.	1.2	17
297	Wavefunction-like Correlation Model for Use in Hybrid Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4590-4599.	2.3	3
298	Combining Wave Function Methods with Density Functional Theory for Excited States. <i>Chemical Reviews</i> , 2018, 118, 7249-7292.	23.0	166
299	Adiabatic Connection without Coupling Constant Integration. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2979-2990.	2.3	14
300	Range-Separated Double-Hybrid Functional from Nonempirical Constraints. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4052-4062.	2.3	45
301	Coordinate Scaling in Time-Independent Excited-State Density Functional Theory for Coulomb Systems. <i>Computation</i> , 2019, 7, 59.	1.0	2
302	Hierarchies of methods towards the exact Kohn-Sham correlation energy based on the adiabatic-connection fluctuation-dissipation theorem. <i>Physical Review B</i> , 2019, 99, .	1.1	35
303	Density Functionals from the Multiple-Radii Approach: Analysis and Recovery of the Kinetic Correlation Energy. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3580-3590.	2.3	7
304	Small Basis Set Allowing the Recovery of Dispersion Interactions with Double-Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2944-2953.	2.3	15
305	A Continuum from Halogen Bonds to Covalent Bonds: Where Do I_3^- Iodanes Fit?. <i>Inorganics</i> , 2019, 7, 47.	1.2	39
306	Correlation energy functionals from adiabatic connection formalism. <i>Physical Review B</i> , 2019, 99, .	1.1	19
307	Improvement of functionals in density functional theory by the inverse Kohnâ€“Sham method and density functional perturbation theory. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2019, 52, 245003.	0.6	11
308	Beyond the RPA and GW methods with adiabatic xc-kernels for accurate ground state and quasiparticle energies. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	33
309	Accurate heats of formation of polycyclic saturated hydrocarbons predicted by using the XYG3 type of doubly hybrid functionals. <i>Journal of Computational Chemistry</i> , 2019, 40, 1113-1122.	1.5	6

#	ARTICLE	IF	CITATIONS
310	How does SCAN compare to PBE in the framework of parameter-free spin-opposite-scaled double-hybrids?. <i>Chemical Physics Letters</i> , 2020, 738, 136898.	1.2	5
311	Density Functional Theories and Coordination Chemistry. , 2020, , .		2
312	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7413-7430.	2.3	12
313	Theoretical analysis of an anion- C_6F_6 complex: $\text{I}^-\cdot\text{C}_6\text{F}_6$. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 285-290.	0.6	3
314	Accurate Hybrid Density Functionals with UW12 Correlation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6176-6194.	2.3	5
315	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
316	MAP: An MP2 Accuracy Predictor for Weak Interactions from Adiabatic Connection Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4141-4149.	2.3	10
317	Improved transition metal surface energies from a generalized gradient approximation developed for quasi two-dimensional systems. <i>Journal of Chemical Physics</i> , 2020, 152, 151101.	1.2	14
318	Exact Generalized Kohn-Sham Theory for Hybrid Functionals. <i>Physical Review X</i> , 2020, 10, .	2.8	19
319	Inverse Kohn-Sham Equations Derived from the Density Equation Theory. <i>Journal of the Physical Society of Japan</i> , 2020, 89, 024301.	0.7	1
320	Screening nature of the van der Waals density functional method: a review and analysis of the many-body physics foundation. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 393001.	0.7	28
321	Modified Interaction-Strength Interpolation Method as an Important Step toward Self-Consistent Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4983-4992.	2.3	14
322	Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states. <i>Journal of Computational Chemistry</i> , 2020, 41, 1242-1251.	1.5	42
323	Divergence of Many-Body Perturbation Theory for Noncovalent Interactions of Large Molecules. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2258-2273.	2.3	39
324	Appraising spin-state energetics in transition metal complexes using double-hybrid models: accountability of SOS0-PBESCAN0-2(a) as a promising paradigm. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9388-9404.	1.3	10
325	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of SIE and NCE . <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, .	6.2	25
326	The Trip to the Density Functional Theory Zoo Continues: Making a Case for Time-Dependent Double Hybrids for Excited-State Problems. <i>Australian Journal of Chemistry</i> , 2021, 74, 3.	0.5	39
327	Prediction of Heats of Formation of Polycyclic Saturated Hydrocarbons Using the XYG3 Double Hybrid Functionals. <i>Springer Series in Materials Science</i> , 2021, , 245-255.	0.4	1

#	ARTICLE	IF	CITATIONS
328	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. <i>Journal of Chemical Physics</i> , 2021, 154, 061101.	1.2	70
329	Relativistic density-functional theory based on effective quantum electrodynamics. , 2021, 1, .		5
330	Noncovalent Interactions from Models for the MÅllerâ€Plesset Adiabatic Connection. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4867-4875.	2.1	15
331	Improving the applicability of the Pauli kinetic energy density based semilocal functional for solids. <i>New Journal of Physics</i> , 2021, 23, 063007.	1.2	13
332	Spin-Opposite-Scaled Range-Separated Exchange Double-Hybrid Models (SOS-RSX-DHs): Marriage Between DH and RSX/SOS-RSX Is Not Always a Happy Match. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4077-4091.	2.3	7
333	Assessing locally range-separated hybrid functionals from a gradient expansion of the exchange energy density. <i>Journal of Chemical Physics</i> , 2021, 154, 214101.	1.2	10
334	Quasi-dimensional models applied to kinetic and exchange energy density functionals. <i>European Physical Journal B</i> , 2021, 94, 1.	0.6	0
335	vdW-DF-ahcx: a range-separated van der Waals density functional hybrid. <i>Journal of Physics Condensed Matter</i> , 2021, 34, .	0.7	7
336	Localization via Density Functionals. <i>Topics in Current Chemistry</i> , 1999, , 201-230.	4.0	1
337	Thomas-Fermi and Other Density-Functional Theories. , 2006, , 295-306.		4
338	On Time-Independent Density-Functional Theories for Excited States. , 1999, , 299-308.		2
339	A Correlation-Energy Functional for Addition to the Hartree-Fock Energy. , 1998, , 133-147.		2
340	Mixing Exact Exchange with GGA: When to Say When. , 1998, , 57-68.		32
342	A New Generation of Doubly Hybrid Density Functionals (DHDFs). <i>Springer Briefs in Molecular Science</i> , 2014, , 25-45.	0.1	2
343	Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response. <i>Journal of Chemical Physics</i> , 2020, 152, 044111.	1.2	22
344	Correlation Energy Contributions from Low-lying States to Density Functionals in the KLI Approximation. <i>Progress in Theoretical Chemistry and Physics</i> , 2001, , 25-44.	0.2	0
345	Theory of Exact Exchange Relations for a Single Excited State. <i>Progress in Theoretical Chemistry and Physics</i> , 2001, , 13-24.	0.2	0
346	Can Density Functional Theory Describe Strongly Correlated Electronic Systems?. , 2002, , 237-252.		2

#	ARTICLE	IF	CITATIONS
348	Unconstrained Variational Determination of the Kohn-Sham Potential. , 2006, , 1469-1472.		0
349	Electron correlation methods based on the random phase approximation. , 2012, , 103-120.		0
350	Benchmarking the Performance of DHDFs for the Main Group Chemistry. Springer Briefs in Molecular Science, 2014, , 47-77.	0.1	0
351	Brief Introduction to Density Functional Theory. , 1998, , 3-18.		1
352	Correlation Energy in a High-Density Limit from Adiabatic Connection Perturbation Theory. , 1998, , 113-123.		0
354	A Brief Report on Density Functional Theory. , 1999, , 47-58.		0
355	Second-order perturbative correlation energy functional in the ensemble density-functional theory. Physical Review A, 2021, 104, .	1.0	2
356	Generalised Kohn-Sham equations with accurate total energy and single-particle eigenvalue spectrum. Journal of Chemical Physics, 2021, 155, 224105.	1.2	3
357	Readdressing molecular dissociation within the Kohn-Sham formalism of density-functional theory: simple models and a different point of view. Molecular Physics, 0, , .	0.8	0
358	Dispersion size-consistency. Electronic Structure, 2022, 4, 014003.	1.0	3
359	Do any types of double-hybrid models render the correct order of excited state energies in inverted singlet-triplet emitters?. Journal of Chemical Physics, 2022, 156, 064302.	1.2	6
360	A general justification for hybrid functionals in DFT by means of linear response theory*. Journal of Physics Condensed Matter, 2022, 34, 194004.	0.7	0
361	Tension between predicting accurate ground state correlation energies and excitation energies from adiabatic approximations in TDDFT. Journal of Chemical Physics, 2022, 156, 084116.	1.2	0
362	Gradient Expansions for the Large-Coupling Strength Limit of the Plesset Adiabatic Connection. Journal of Chemical Theory and Computation, 2022, 18, 1584-1594.	2.3	11
363	Boosting the OEP2-sc method with spin-component scaling. Molecular Physics, 2022, 120, .	0.8	2
364	Electronic Structure of (Organic)Inorganic Metal Halide Perovskites: The Dilemma of Choosing the Right Functional. Advanced Theory and Simulations, 2022, 5, .	1.3	9
365	Double and Charge-Transfer Excitations in Time-Dependent Density Functional Theory. Annual Review of Physical Chemistry, 2022, 73, 117-140.	4.8	23
367	Workhorse minimally empirical dispersion-corrected density functional with tests for weakly bound systems: $\text{SCAN}+r_2$ Physical Review B, 2022, 106, .	1.1	18

#	ARTICLE	IF	CITATIONS
368	Benchmarking time-dependent density functional theory for singlet excited states of thermally activated delayed fluorescence chromophores. <i>Physical Review Research</i> , 2022, 4, .	1.3	10
369	Comparing correlation components and approximations in Hartree-Fock and Kohn-Sham theories via an analytical test case study. <i>Journal of Chemical Physics</i> , 2022, 157, 054102.	1.2	3
370	Density functionals based on the mathematical structure of the strong-interaction limit of <i>DFT</i> . <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, .	6.2	11
371	Reduced density matrix functional theory from an <i>ab initio</i> seniority-zero wave function: Exact and approximate formulations along adiabatic connection paths. <i>Physical Review A</i> , 2022, 106, .	1.0	7
372	<i>Kohn-Sham</i> potentials by an inverse <i>Kohn-Sham</i> equation and accuracy assessment by virial theorem. <i>Journal of the Chinese Chemical Society</i> , 2023, 70, 554-569.	0.8	3
373	Inversion Theory Leveling as a New Methodological Approach to Antioxidant Thermodynamics: A Case Study on Phenol. <i>Antioxidants</i> , 2023, 12, 282.	2.2	0
374	Thomas-Fermi and Other Density-Functional Theories. <i>Springer Handbooks</i> , 2023, , 297-308.	0.3	0
375	Electronic Excited States in Extreme Limits via Ensemble Density Functionals. <i>Physical Review Letters</i> , 2023, 130, .	2.9	6
376	Physically meaningful solutions of optimized effective potential equations in a finite basis set within KS-DFT framework. <i>Advances in Quantum Chemistry</i> , 2023, , .	0.4	0
377	The Strong-Interaction Limit of Density Functional Theory. , 2023, , 183-266.		3
378	Review of Approximations for the Exchange-Correlation Energy in Density-Functional Theory. , 2023, , 1-90.		3
382	Non-empirical quadratic-integrand double-hybrid (QIDH) functionals. <i>Annual Reports in Computational Chemistry</i> , 2023, , 87-119.	0.9	0