Density functionals that are one- and two- are not alwa self-interaction-free, as shown for H2+, He2+, LiH+, and

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Citation Report

#	Article	IF	Citations
1	Computing Fukui functions without differentiating with respect to electron number. II. Calculation of condensed molecular Fukui functions. Journal of Chemical Physics, 2007, 126, 224108.	1.2	58
2	Modeling the adiabatic connection in H2. Journal of Chemical Physics, 2007, 126, 244104.	1.2	34
3	Diminished gradient dependence of density functionals: Constraint satisfaction and self-interaction correction. Journal of Chemical Physics, 2007, 126, 244107.	1.2	26
4	Exchange and correlation in open systems of fluctuating electron number. Physical Review A, 2007, 76, .	1.0	140
5	Computing Fukui functions without differentiating with respect to electron number. I. Fundamentals. Journal of Chemical Physics, 2007, 126, 224107.	1.2	61
6	Tests of functionals for systems with fractional electron number. Journal of Chemical Physics, 2007, 126, 154109.	1.2	559
7	Resonating broken symmetry CI approach for ionâ€radical systems: Comparison with UHF, hybridâ€DFT, and CASSCFâ€DFT. International Journal of Quantum Chemistry, 2008, 108, 2966-2977.	1.0	8
8	Optimal operators for Hartreeâ€“Fock exchange from long-range corrected hybrid density functionals. Chemical Physics Letters, 2008, 467, 176-178.	1.2	68
9	Orbital-dependent density functionals: Theory and applications. Reviews of Modern Physics, 2008, 80, 3-60.	16.4	1,069
10	Long-range corrected hybrid density functionals with damped atomâ€“atom dispersion corrections. Physical Chemistry Chemical Physics, 2008, 10, 6615.	1.3	10,464
11	Empirical Corrections to Density Functional Theory Highlight the Importance of Nonbonded Intramolecular Interactions in Alkanes. Journal of Physical Chemistry A, 2008, 112, 11495-11500.	1.1	48
12	Localization and Delocalization Errors in Density Functional Theory and Implications for Band-Gap Prediction. Physical Review Letters, 2008, 100, 146401.	2.9	1,012
13	Fractional charge perspective on the band gap in density-functional theory. Physical Review B, 2008, 77, .	1.1	491
14	Discontinuity of the exchange-correlation potential: Support for assumptions used to find it. Physical Review A, 2008, 77, .	1.0	83
15	Orbital energies and negative electron affinities from density functional theory: Insight from the integer discontinuity. Journal of Chemical Physics, 2008, 129, 044110.	1.2	112
16	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. Physical Review A, 2008, 77, .	1.0	104
17	Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2008, 4, 1849-1868.	2.3	956
18	Insights into Current Limitations of Density Functional Theory. Science, 2008, 321, 792-794.	6.0	2,057

#	Article	IF	Citations
19	Systematic optimization of long-range corrected hybrid density functionals. Journal of Chemical Physics, 2008, 128, 084106.	1.2	2,890
20	A Density Functional Theory for Symmetric Radical Cations from Bonding to Dissociation. Journal of Physical Chemistry A, 2008, 112, 12789-12791.	1.1	45
21	Simple charge-transfer model to explain the electrical response of hydrogen chains. Physical Review A, 2008, 78, .	1.0	20
22	Towards a theoretical description of molecular junctions in the Coulomb blockade regime based on density functional theory. Physical Review B, 2008, 78, .	1.1	21
23	Ab Initio Molecular Dynamics Study of the Solvated OHCl^{â˜’} Complex: Implications for the Atmospheric Oxidation of Chloride Anion to Molecular Chlorine. Journal of Physical Chemistry A, 2008, 112, 4644-4650.	1.1	22
24	Dynamical Optimization for Partition Theory. Journal of Physical Chemistry A, 2008, 112, 571-575.	1.1	2
25	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. Physical Review A, 2008, 78, .	1.0	221
26	Optimized effective potentials from arbitrary basis sets. Journal of Chemical Physics, 2008, 129, 194102.	1.2	39
27	Self-interaction correction and the optimized effective potential. Journal of Chemical Physics, 2008, 129, 014110.	1.2	72
28	The energy-differences based exact criterion for testing approximations to the functional for the kinetic energy of non-interacting electrons. Journal of Physics A: Mathematical and Theoretical, 2008, 41, 055302.	0.7	33
29	Size extensivity of the direct optimized effective potential method. Journal of Chemical Physics, 2008, 128, 114702.	1.2	5
30	Self-interaction correction with Wannier functions. Physical Review B, 2008, 77, .	1.1	33
31	Understanding and correcting the self-interaction error in the electrical response of hydrogen chains. Physical Review A, 2008, 77, .	1.0	52
32	Configuration mixing within the energy density functional formalism: Removing spurious contributions from nondiagonal energy kernels. Physical Review C, 2009, 79, .	1.1	120
33	Reverse engineering in many-body quantum physics: Correspondence between many-body systems and effective single-particle equations. Physical Review A, 2009, 79, .	1.0	17
34	Comment on â€œFunctional derivative of the universal density functional in Fock spaceâ€• Physical Review A, 2009, 79, .	1.0	17
36	Constrained density functional theory based configuration interaction improves the prediction of reaction barrier heights. Journal of Chemical Physics, 2009, 130, 034109.	1.2	79
37	The self-interaction error and the description of non-dynamic electron correlation in density functional theory. Theoretical Chemistry Accounts, 2009, 123, 171-182.	0.5	51

#	Article	IF	Citations
38	Resonating coupledâ€cluster CI approach to ionâ€radical systems: Comparison with the unrestricted coupledâ€cluster approach. International Journal of Quantum Chemistry, 2009, 109, 3811-3818.	1.0	7
39	A resonating broken-symmetry CI study of cationic states of phenalenyl dimeric compounds. Polyhedron, 2009, 28, 1628-1633.	1.0	4
40	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. Chemical Physics Letters, 2009, 478, 283-286.	1.2	9
41	Electronic Hyperpolarizabilities for Donorâ"Acceptor Molecules with Long Conjugated Bridges: Calculations versus Experiment. Journal of Physical Chemistry A, 2009, 113, 10994-11001.	1.1	129
42	Deleterious Effects of Long-Range Self-Repulsion on the Density Functional Description of O₂ Sticking on Aluminum. Journal of Physical Chemistry A, 2009, 113, 7521-7527.	1.1	27
43	DFT Calculations on Charge-Transfer States of a Carotenoid-Porphyrin-C₆₀ Molecular Triad. Journal of Chemical Theory and Computation, 2009, 5, 834-843.	2.3	62
44	Evaluation of Range-Separated Hybrid and Other Density Functional Approaches on Test Sets Relevant for Transition Metal-Based Homogeneous Catalysts. Journal of Physical Chemistry A, 2009, 113, 11742-11749.	1.1	50
45	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
46	The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems. Journal of Chemical Physics, 2009, 130, 104111.	1.2	64
47	Long-range corrected double-hybrid density functionals. Journal of Chemical Physics, 2009, 131, 174105.	1.2	327
48	Particle-number restoration within the energy density functional formalism. Physical Review C, 2009, 79, .	1.1	118
49	A resonating broken symmetry configuration interaction approach for double-exchange magnetic systems. Journal of Physics Condensed Matter, 2009, 21, 064227.	0.7	8
50	Koopmansâ€™ springs to life. Journal of Chemical Physics, 2009, 131, 231101.	1.2	184
51	An improved long-range corrected hybrid functional with vanishing Hartreeâ€"Fock exchange at zero interelectronic distance (LC2gau-BOP). Journal of Chemical Physics, 2009, 131, 144108.	1.2	45
52	Chemical Reactivity Descriptors for Ambiphilic Reagents: Dual Descriptor, Local Hypersoftness, and Electrostatic Potential. Journal of Physical Chemistry A, 2009, 113, 8660-8667.	1.1	166
53	Second-Order Perturbation Theory with Fractional Charges and Fractional Spins. Journal of Chemical Theory and Computation, 2009, 5, 786-792.	2.3	61
54	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. Molecular Physics, 2009, 107, 1077-1088.	0.8	17
55	Physical signatures of discontinuities of the time-dependent exchangeâ€"correlation potential. Physical Chemistry Chemical Physics, 2009, 11, 4647.	1.3	22

#	Article	IF	Citations
56	Reaction Enthalpies Using the Neural-Network-Based X1 Approach: The Important Choice of Input Descriptors. Journal of Physical Chemistry A, 2009, 113, 3285-3290.	1.1	19
57	Overcoming systematic DFT errors for hydrocarbon reaction energies. Theoretical Chemistry Accounts, 2010, 127, 429-442.	0.5	51
58	Fourteen easy lessons in density functional theory. International Journal of Quantum Chemistry, 2010, 110, 2801-2807.	1.0	41
59	Dimensionality dependence of the self-interaction correction in the local-density approximation to density functional theory. Physical Review B, 2010, 81, .	1.1	3
60	Hybrid functionals including random phase approximation correlation and second-order screened exchange. Journal of Chemical Physics, 2010, 132, 094103.	1.2	131
61	Subsystem constraints in variational second order density matrix optimization: Curing the dissociative behavior. Journal of Chemical Physics, 2010, 132, 114113.	1.2	41
62	Many-electron self-interaction and spin polarization errors in local hybrid density functionals. Journal of Chemical Physics, 2010, 133, 134116.	1.2	83
63	Global Hybrid Functionals: A Look at the Engine under the Hood. Journal of Chemical Theory and Computation, 2010, 6, 3688-3703.	2.3	87
64	A General Database for Main Group Thermochemistry, Kinetics, and Noncovalent Interactions â˜' Assessment of Common and Reparameterized (meta-)GGA Density Functionals. Journal of Chemical Theory and Computation, 2010, 6, 107-126.	2.3	389
65	Magnetizabilities at Self-Interaction-Corrected Density Functional Theory Level. Journal of Chemical Theory and Computation, 2010, 6, 3302-3311.	2.3	10
66	Tuned Range-Separated Hybrids in Density Functional Theory. Annual Review of Physical Chemistry, 2010, 61, 85-109.	4.8	661
67	Density Functional Theory of Electronic Structure: A Short Course for Mineralogists and Geophysicists. Reviews in Mineralogy and Geochemistry, 2010, 71, 1-18.	2.2	16
68	Koopmansâ€™ condition for density-functional theory. Physical Review B, 2010, 82, .	1.1	206
69	The RPA Atomization Energy Puzzle. Journal of Chemical Theory and Computation, 2010, 6, 127-134.	2.3	76
70	TD-CI Simulation of the Electronic Optical Response of Molecules in Intense Fields II: Comparison of DFT Functionals and EOM-CCSD. Journal of Physical Chemistry A, 2011, 115, 11832-11840.	1.1	42
71	Reactivity indicators for degenerate states in the density-functional theoretic chemical reactivity theory. Journal of Chemical Physics, 2011, 134, 174103.	1.2	74
72	Electronic hole transfer in rutile and anatase TiO2: Effect of a delocalization error in the density functional theory on the charge transfer barrier height. Physical Review B, 2011, 84, .	1.1	14
75	Accurate Dispersion-Corrected Density Functionals for General Chemistry Applications. , 2011, , 1-16.		2

#	Article	IF	Citations
76	Evaluating the Performance of DFT Functionals in Assessing the Interaction Energy and Ground-State Charge Transfer of Donor/Acceptor Complexes: Tetrathiafulvaleneâ"Tetracyanoquinodimethane (TTFâ"TCNQ) as a Model Case. Journal of Chemical Theory and Computation, 2011, 7, 602-609.	2.3	143
77	A Density Functional Theory for Studying Ionization Processes in Water Clusters. Journal of Physical Chemistry A, 2011, 115, 5735-5744.	1.1	51
78	Comparative study of hybrid functionals applied to structural and electronic properties of semiconductors and insulators. Physical Review B, 2011, 84, .	1.1	67
79	Benchmark results for empirical post-GGA functionals: Difficult exchange problems and independent tests. Physical Chemistry Chemical Physics, 2011, 13, 19325.	1.3	83
80	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. Physical Chemistry Chemical Physics, 2011, 13, 6670.	1.3	1,627
81	Dispersion, static correlation, and delocalisation errors in density functional theory: An electrostatic theorem perspective. Journal of Chemical Physics, 2011, 135, 164110.	1.2	10
82	Density Functional Theory for Reaction Energies: Test of Meta and Hybrid Meta Functionals, Range-Separated Functionals, and Other High-Performance Functionals. Journal of Chemical Theory and Computation, 2011, 7, 669-676.	2.3	190
83	Twelve outstanding problems in ground-state density functional theory: A bouquet of puzzles. Computational and Theoretical Chemistry, 2011, 963, 2-6.	1.1	43
84	Non-empirical improvement of PBE and its hybrid PBE0 for general description of molecular properties. Journal of Chemical Physics, 2012, 136, 104108.	1.2	78
85	Long-range corrected hybrid meta-generalized-gradient approximations with dispersion corrections. Journal of Chemical Physics, 2012, 136, 154109.	1.2	101
86	Importance of the correlation contribution for local hybrid functionals: Range separation and self-interaction corrections. Journal of Chemical Physics, 2012, 136, 014111.	1.2	83
87	Using complex degrees of freedom in the Kohn-Sham self-interaction correction. Physical Review A, 2012, 85, .	1.0	50
88	Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains. Journal of Chemical Physics, 2012, 137, 214106.	1.2	66
89	ELEMENTAL AND MIXED ACTINIDE DIOXIDES: AN AB INITIO STUDY. Journal of Theoretical and Computational Chemistry, 2012, 11, 611-629.	1.8	11
90	Oxidative trends of TiO2â€"hole trapping at anatase and rutile surfaces. Energy and Environmental Science, 2012, 5, 9866.	15.6	41
91	Curvature and Frontier Orbital Energies in Density Functional Theory. Journal of Physical Chemistry Letters, 2012, 3, 3740-3744.	2.1	145
92	Attenuating Away the Errors in Inter- and Intramolecular Interactions from Second-Order MÃ¸llerâ€"Plesset Calculations in the Small Aug-cc-pVDZ Basis Set. Journal of Physical Chemistry Letters, 2012, 3, 3592-3598.	2.1	34
93	Self-interaction correction scheme for approximate Kohn-Sham potentials. Physical Review A, 2012, 86, .	1.0	17

#	Article	IF	Citations
94	Self-interaction correction to GW approximation. Physica Scripta, 2012, 86, 065301.	1.2	4
95	Symmetric Nonlocal Weighted Density Approximations from the Exchange-Correlation Hole of the Uniform Electron Gas. Journal of Chemical Theory and Computation, 2012, 8, 4081-4093.	2.3	22
96	Magnetic Exchange Couplings from Semilocal Functionals Evaluated Nonself-Consistently on Hybrid Densities: Insights on Relative Importance of Exchange, Correlation, and Delocalization. Journal of Chemical Theory and Computation, 2012, 8, 3147-3158.	2.3	34
97	Constrained Density Functional Theory. Chemical Reviews, 2012, 112, 321-370.	23.0	454
98	Comparison of the performance of exact-exchange-based density functional methods. Journal of Chemical Physics, 2012, 137, 114104.	1.2	33
99	Derivative discontinuity, bandgap and lowest unoccupied molecular orbital in density functional theory. Journal of Chemical Physics, 2012, 136, 204111.	1.2	154
100	Exploring the Limits of Density Functional Approximations for Interaction Energies of Molecular Precursors to Organic Electronics. Journal of Chemical Theory and Computation, 2012, 8, 4305-4316.	2.3	38
101	Switchable Nonlinear Optical Properties of Î·⁵-Monocyclopentadienylmetal Complexes: A DFT Approach. Journal of Chemical Information and Modeling, 2012, 52, 1970-1983.	2.5	20
102	The benchmark of Gutzwiller density functional theory in hydrogen systems. International Journal of Quantum Chemistry, 2012, 112, 240-246.	1.0	5
103	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2012, 8, 1515-1531.	2.3	765
104	Challenges for Density Functional Theory. Chemical Reviews, 2012, 112, 289-320.	23.0	1,869
105	Calculation of dispersion energies. Journal of Physics Condensed Matter, 2012, 24, 073201.	0.7	187
106	A variational principle for the electron density using the exchange hole & its implications for N-representability. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 839-844.	0.9	6
108	Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. Physical Review Letters, 2013, 111, 106401.	2.9	168
109	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, , 1-57.		1
110	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
111	Long-Range Corrected Hybrid Density Functionals with Improved Dispersion Corrections. Journal of Chemical Theory and Computation, 2013, 9, 263-272.	2.3	535
112	Longâ€range corrected functionals satisfy Koopmans' theorem: Calculation of correlation and relaxation energies. Journal of Computational Chemistry, 2013, 34, 958-964.	1.5	65

#	Article	IF	Citations
113	Assessment of density functional methods with correct asymptotic behavior. Physical Chemistry Chemical Physics, 2013, 15, 8352.	1.3	49
114	H Atom Adsorption on a Silicate Surface: The (010) Surface of Forsterite. Journal of Physical Chemistry C, 2013, 117, 12612-12621.	1.5	27
115	The Performance of Density Functionals for Sulfateâ€“Water Clusters. Journal of Chemical Theory and Computation, 2013, 9, 1368-1380.	2.3	69
116	Assessment of Tuning Methods for Enforcing Approximate Energy Linearity in Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2013, 9, 4414-4420.	2.3	31
117	Massively parallel implementations of coupled-cluster methods for electron spin resonance spectra. I. Isotropic hyperfine coupling tensors in large radicals. Journal of Chemical Physics, 2013, 139, 174103.	1.2	16
118	Extreme density-driven delocalization error for a model solvated-electron system. Journal of Chemical Physics, 2013, 139, 184116.	1.2	93
119	Piecewise Linearity of Approximate Density Functionals Revisited: Implications for Frontier Orbital Energies. Physical Review Letters, 2013, 110, 126403.	2.9	110
120	Point-defect optical transitions and thermal ionization energies from quantum Monte Carlo methods: Application to the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>F</mml:mi></mml:math>-center defect in MgO. Physical Review B, 2013, 87, .	1.1	53
121	Fundamental gaps with approximate density functionals: The derivative discontinuity revealed from ensemble considerations. Journal of Chemical Physics, 2014, 140, 18A540.	1.2	75
122	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. Journal of Chemical Physics, 2014, 140, 18A538.	1.2	10
123	Local-hybrid functional based on the correlation length. Journal of Chemical Physics, 2014, 141, 124120.	1.2	38
124	Kohn-Sham potentials in exact density-functional theory at noninteger electron numbers. Physical Review A, 2014, 90, .	1.0	42
125	Tight constraints on the exchange-correlation potentials of degenerate states. Journal of Chemical Physics, 2014, 140, 18A537.	1.2	6
126	25th Anniversary Article: Design of Polymethine Dyes for Allâ€Optical Switching Applications: Guidance from Theoretical and Computational Studies. Advanced Materials, 2014, 26, 68-84.	11.1	97
127	Correlation matrix renormalization approximation for total-energy calculations of correlated electron systems. Physical Review B, 2014, 89, .	1.1	15
128	Qualitative breakdown of the unrestricted Hartree-Fock energy. Journal of Chemical Physics, 2014, 141, 164124.	1.2	9
129	Atomic electron affinities and the role of symmetry between electron addition and subtraction in a corrected Koopmans approach. Physical Chemistry Chemical Physics, 2014, 16, 14420-14434.	1.3	9
130	Quantum-chemical insights into mixed-valence systems: within and beyond the Robinâ€“Day scheme. Chemical Society Reviews, 2014, 43, 5067-5088.	18.7	168

#	Article	IF	Citations
131	Ping-Pong Protons: How Hydrogen-Bonding Networks Facilitate Heterolytic Bond Cleavage in Peptide Radical Cations. Journal of Physical Chemistry B, 2014, 118, 2628-2637.	1.2	7
132	Reactions of Methanol with Pristine and Defective Ceria (111) Surfaces: A Comparison of Density Functionals. Journal of Physical Chemistry C, 2014, 118, 23690-23700.	1.5	33
133	On a solution of the self-interaction problem in Kohnâ€“Sham density functional theory. Journal of Physics and Chemistry of Solids, 2014, 75, 1160-1178.	1.9	9
134	High-resolution spectroscopy and quantum-defect model for the gerade triplet np and nf Rydberg states of He2. Journal of Chemical Physics, 2014, 140, 064304.	1.2	11
135	Insight into organic reactions from the direct random phase approximation and its corrections. Journal of Chemical Physics, 2015, 143, 144115.	1.2	11
136	Effect of ensemble generalization on the highest-occupied Kohn-Sham eigenvalue. Journal of Chemical Physics, 2015, 143, 104105.	1.2	16
137	Integer versus Fractional Charge Transfer at Metal(/Insulator)/Organic Interfaces: Cu(/NaCl)/TCNE. ACS Nano, 2015, 9, 5391-5404.	7.3	58
138	New massively parallel linear-response coupled-cluster module in ACES III: application to static polarisabilities of closed-shell molecules and oligomers and of open-shell radicals. Molecular Physics, 0, , 1-15.	0.8	1
139	Deviations from piecewise linearity in the solid-state limit with approximate density functionals. Journal of Chemical Physics, 2015, 142, 034107.	1.2	42
140	Accurate Dielsâ€“Alder Reaction Energies from Efficient Density Functional Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2879-2888.	2.3	19
141	Variational minimization of orbital-density-dependent functionals. Physical Review B, 2015, 91, .	1.1	29
142	Elimination of the asymptotic fractional dissociation problem in Kohn-Sham density-functional theory using the ensemble-generalization approach. Physical Review A, 2015, 91, .	1.0	26
143	Fractional Electron Loss in Approximate DFT and Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2015, 11, 5262-5268.	2.3	38
144	The effect of nitrido, azide, and nitrosyl ligands on magnetization densities and magnetic properties of iridium PNP pincer-type complexes. RSC Advances, 2015, 5, 84311-84320.	1.7	1
145	Fractional charge and spin errors in self-consistent Greenâ€™s function theory. Journal of Chemical Physics, 2015, 142, 194108.	1.2	37
146	Size-dependent properties of transition metal clusters: from molecules to crystals and surfaces â€“ computational studies with the program ParaGauss. Physical Chemistry Chemical Physics, 2015, 17, 28463-28483.	1.3	16
147	System-dependent exchangeâ€“correlation functional with exact asymptotic potential and ÎµHOMO â‰ˆ â^’ I. Journal of Chemical Physics, 2015, 143, 024104.	1.2	13
148	Scaling correction approaches for reducing delocalization error in density functional approximations. Science China Chemistry, 2015, 58, 1825-1844.	4.2	12

#	Article	IF	Citations
149	Alternative Ornsteinâ€“Zernike models from the homogeneous electron liquid for density functional theory calculations. International Journal of Quantum Chemistry, 2016, 116, 852-861.	1.0	3
150	SCAN-based hybrid and double-hybrid density functionals from models without fitted parameters. Journal of Chemical Physics, 2016, 144, 044114.	1.2	126
151	Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. Journal of Chemical Physics, 2016, 145, 204101.	1.2	26
152	Ionisation potential theorem in the presence of the electric field: Assessment of range-separated functional in the reproduction of orbital and excitation energies. Journal of Chemical Physics, 2016, 144, 164113.	1.2	6
153	Global and local curvature in density functional theory. Journal of Chemical Physics, 2016, 145, 054109.	1.2	38
154	Hybrid Density Functionals Applied to Complex Solid Catalysts: Successes, Limitations, and Prospects. Catalysis Letters, 2016, 146, 861-885.	1.4	31
155	Complex Orbitals, Multiple Local Minima, and Symmetry Breaking in Perdewâ€“Zunger Self-Interaction Corrected Density Functional Theory Calculations. Journal of Chemical Theory and Computation, 2016, 12, 3195-3207.	2.3	54
156	Potential Dependence of Electrochemical Barriers from ab Initio Calculations. Journal of Physical Chemistry Letters, 2016, 7, 1686-1690.	2.1	213
157	How Large Should the QM Region Be in QM/MM Calculations? The Case of Catechol O-Methyltransferase. Journal of Physical Chemistry B, 2016, 120, 11381-11394.	1.2	150
158	Kineticâ€energyâ€density dependent semilocal exchangeâ€correlation functionals. International Journal of Quantum Chemistry, 2016, 116, 1641-1694.	1.0	78
159	Effect of Complex-Valued Optimal Orbitals on Atomization Energies with the Perdewâ€“Zunger Self-Interaction Correction to Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 4296-4302.	2.3	29
160	Systematic treatment of spin-reactivity indicators in conceptual density functional theory. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	16
161	Barriers of Electrochemical CO₂ Reduction on Transition Metals. Organic Process Research and Development, 2016, 20, 1424-1430.	1.3	135
162	One- and many-electron self-interaction error in local and global hybrid functionals. Physical Review B, 2016, 93, .	1.1	62
163	Where Does the Density Localize? Convergent Behavior for Global Hybrids, Range Separation, and DFT+U. Journal of Chemical Theory and Computation, 2016, 12, 5931-5945.	2.3	65
164	Kohn-Sham potential for a strongly correlated finite system with fractional occupancy. Physical Review A, 2016, 94, .	1.0	23
165	Communication: Two types of flat-planes conditions in density functional theory. Journal of Chemical Physics, 2016, 145, 031102.	1.2	22
166	Ill-advised self-interaction contribution in modelling anionic attack along a reaction path. Molecular Physics, 2016, 114, 1066-1075.	0.8	3

#	Article	IF	Citations
167	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods. Journal of Chemical Theory and Computation, 2016, 12, 615-626.	2.3	154
168	Implementation of a Parallel Linear-Response Coupled-Cluster-Theory Module in ACES III. Advances in Quantum Chemistry, 2016, , 29-60.	0.4	3
169	Accurate description of the electronic structure of organic semiconductors byGWmethods. Journal of Physics Condensed Matter, 2017, 29, 103003.	0.7	26
170	Vibrational Frequencies of Fractionally Charged Molecular Species: Benchmarking DFT Results against ab Initio Calculations. Journal of Physical Chemistry A, 2017, 121, 2282-2287.	1.1	4
171	Does the ionization potential condition employed in QTP functionals mitigate the self-interaction error?. Journal of Chemical Physics, 2017, 146, 034102.	1.2	22
172	Comparing the performance of TDâ€ĐFT and SACâ€CI methods in the description of excited states potential energy surfaces: An excited state proton transfer reaction as case study. Journal of Computational Chemistry, 2017, 38, 1084-1092.	1.5	15
173	Density functional theory for modelling large molecular adsorbateâ€“surface interactions: a mini-review and worked example. Molecular Simulation, 2017, 43, 327-345.	0.9	39
174	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2017, 13, 441-450.	2.3	56
175	Unifying Exchange Sensitivity in Transition-Metal Spin-State Ordering and Catalysis through Bond Valence Metrics. Journal of Chemical Theory and Computation, 2017, 13, 5443-5457.	2.3	43
176	The ionic versus metallic nature of 2D electrides: a density-functional description. Physical Chemistry Chemical Physics, 2017, 19, 27343-27352.	1.3	16
177	A new nonempirical tuning scheme with single selfâ€consistent field calculation: Comparison with global and IPâ€tuned rangeâ€separated functional. Journal of Computational Chemistry, 2017, 38, 2258-2267.	1.5	18
178	Multiconfiguration Pair-Density Functional Theory Is Free From Delocalization Error. Journal of Physical Chemistry Letters, 2017, 8, 5616-5620.	2.1	31
179	Fractional-charge and fractional-spin errors in range-separated density-functional theory. Molecular Physics, 2017, 115, 161-173.	0.8	21
180	Vibrational properties of fractionally charged molecules and their relevance for molecular electronics and electrochemistry. Chemical Physics, 2017, 482, 311-318.	0.9	6
181	Communication: Recovering the flat-plane condition in electronic structure theory at semi-local DFT cost. Journal of Chemical Physics, 2017, 147, 191101.	1.2	34
182	A meta-GGA level screened range-separated hybrid functional by employing short range Hartreeâ€“Fock with a long range semilocal functional. Physical Chemistry Chemical Physics, 2018, 20, 8999-9005.	1.3	21
183	Self-Interaction Error in Density Functional Theory: An Appraisal. Journal of Physical Chemistry Letters, 2018, 9, 2353-2358.	2.1	131
184	Free Energy Profile of NaCl in Water: First-Principles Molecular Dynamics with SCAN and Ï‰B97X-V Exchangeâ€“Correlation Functionals. Journal of Chemical Theory and Computation, 2018, 14, 884-893.	2.3	41

#	Article	IF	Citations
185	Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. National Science Review, 2018, 5, 203-215.	4.6	110
186	Where Does the Density Localize in the Solid State? Divergent Behavior for Hybrids and DFT+U. Journal of Chemical Theory and Computation, 2018, 14, 670-683.	2.3	57
187	Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes. Journal of Physical Chemistry A, 2018, 122, 4219-4245.	1.1	97
188	Shrinking Self-Interaction Errors with the Fermiâ€“LÃ¶wdin Orbital Self-Interaction-Corrected Density Functional Approximation. Journal of Physical Chemistry A, 2018, 122, 9307-9315.	1.1	30
189	On the many-electron self-interaction error of the semilocal exchange hole based meta-GGA level range-separated hybrid with the B88 hybrids. Chemical Physics Letters, 2018, 713, 1-9.	1.2	17
190	Performance and Scope of Perturbative Corrections to Random-Phase Approximation Energies. Journal of Chemical Theory and Computation, 2018, 14, 5701-5714.	2.3	23
191	Fermiâ€Ã¶wdin orbital selfâ€interaction corrected density functional theory: Ionization potentials and enthalpies of formation. Journal of Computational Chemistry, 2018, 39, 2463-2471.	1.5	35
192	Delocalization Errors in Density Functional Theory Are Essentially Quadratic in Fractional Occupation Number. Journal of Physical Chemistry Letters, 2018, 9, 6280-6288.	2.1	71
193	Theoretical Descriptors of Electrides. Journal of Physical Chemistry A, 2018, 122, 9371-9391.	1.1	63
194	Describing strong correlation with fractional-spin correction in density functional theory. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9678-9683.	3.3	56
195	How well can density functional theory and pair-density functional theory predict the correct atomic charges for dissociation and accurate dissociation energetics of ionic bonds?. Physical Chemistry Chemical Physics, 2018, 20, 23072-23078.	1.3	11
196	Density functional approximations for orbital energies and total energies of molecules and solids. Journal of Chemical Physics, 2018, 149, 054105.	1.2	29
197	From semilocal density functionals to random phase approximation renormalized perturbation theory: A methodological assessment of structural phase transitions. Physical Review B, 2018, 97, .	1.1	68
198	Stable Surfaces That Bind Too Tightly: Can Range-Separated Hybrids or DFT+U Improve Paradoxical Descriptions of Surface Chemistry?. Journal of Physical Chemistry Letters, 2019, 10, 5090-5098.	2.1	27
199	Beyond Density Functional Theory: The Multiconfigurational Approach To Model Heterogeneous Catalysis. ACS Catalysis, 2019, 9, 8481-8502.	5.5	75
200	Computational Exploration of NO Single-Site Disproportionation on Fe-MOF-5. Chemistry of Materials, 2019, 31, 8875-8885.	3.2	20
201	Exploring local range separation: The role of spin scaling and one-electron self-interaction. Journal of Chemical Physics, 2019, 151, 154108.	1.2	11
202	Implementation of the Many-Pair Expansion for Systematically Improving Density Functional Calculations of Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1089-1101.	2.3	5

#	Article	IF	Citations
203	Non-empirical, low-cost recovery of exact conditions with model-Hamiltonian inspired expressions in jmDFT. Journal of Chemical Physics, 2019, 150, 154115.	1.2	13
204	Long-range screened hybrid-functional theory satisfying the local-density linear response. Physical Review A, 2019, 99, .	1.0	16
205	TDDFT+U : A critical assessment of the Hubbard U correction to exchange-correlation kernels and potentials. Physical Review B, 2019, 99, .	1.1	8
206	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
207	Impact of Approximate DFT Density Delocalization Error on Potential Energy Surfaces in Transition Metal Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 264-277.	2.3	22
208	Benchmarking an Embedded Adaptive Sampling Configuration Interaction Method for Surface Reactions: H₂ Desorption from and CH₄ Dissociation on Cu(111). Journal of Chemical Theory and Computation, 2020, 16, 7078-7088.	2.3	23
209	Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic U. Physical Review B, 2020, 102, .	1.1	48
210	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. Journal of Chemical Theory and Computation, 2020, 16, 7413-7430.	2.3	12
211	Electronic and Optical Properties of Protonated Triazine Derivatives. Journal of Physical Chemistry C, 2020, 124, 27801-27810.	1.5	5
212	Large-scale comparison of 3d and 4d transition metal complexes illuminates the reduced effect of exchange on second-row spin-state energetics. Physical Chemistry Chemical Physics, 2020, 22, 19326-19341.	1.3	20
213	Lysosome Targeting Bis-terpyridine Ruthenium(II) Complexes: Photophysical Properties and In Vitro Photodynamic Therapy. ACS Applied Bio Materials, 2020, 3, 6025-6038.	2.3	29
214	The one-electron self-interaction error in 74 density functional approximations: a case study on hydrogenic mono- and dinuclear systems. Physical Chemistry Chemical Physics, 2020, 22, 15805-15830.	1.3	27
215	Machine learning models of the energy curvature vs particle number for optimal tuning of long-range corrected functionals. Journal of Chemical Physics, 2020, 152, 154103.	1.2	12
216	First-principles Hubbard <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> and Hund's <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>J</mml:mi></mml:math> corrected approximate density functional theory predicts an accurate fundamental gap in rutile and anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml	1.1	31
217	Improvements in the orbitalwise scaling down of Perdewâ€“Zunger self-interaction correction in many-electron regions. Journal of Chemical Physics, 2020, 152, 174112.	1.2	23
218	Preserving Symmetry and Degeneracy in the Localized Orbital Scaling Correction Approach. Journal of Physical Chemistry Letters, 2020, 11, 1528-1535.	2.1	31
219	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of <scp>SIE</scp> and <scp>NCE</scp>. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, .	6.2	25
220	Local self-interaction correction method with a simple scaling factor. Physical Chemistry Chemical Physics, 2021, 23, 2406-2418.	1.3	14

#	Article	IF	Citations
221	Challenges for density functional theory: calculation of CO adsorption on electrocatalytically relevant metals. Physical Chemistry Chemical Physics, 2021, 23, 9394-9406.	1.3	15
222	The Role of Range-Separated Correlation in Long-Range Corrected Hybrid Functionals. Journal of Physical Chemistry Letters, 2021, 12, 1207-1213.	2.1	7
223	Replacing hybrid density functional theory: motivation and recent advances. Chemical Society Reviews, 2021, 50, 8470-8495.	18.7	80
224	Self-Interaction-Corrected Random Phase Approximation. Journal of Chemical Theory and Computation, 2021, 17, 2107-2115.	2.3	2
225	Exploring and enhancing the accuracy of interior-scaled Perdewâ€“Zunger self-interaction correction. Journal of Chemical Physics, 2021, 154, 094105.	1.2	12
226	Molecular DFT+U: A Transferable, Low-Cost Approach to Eliminate Delocalization Error. Journal of Physical Chemistry Letters, 2021, 12, 3633-3640.	2.1	9
227	Fermi-LÃ¶wdin-orbital self-interaction correction using the optimized-effective-potential method within the Krieger-Li-Iafrate approximation. Physical Review A, 2021, 103, .	1.0	14
228	Correcting the Charge Delocalization Error of Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 4633-4638.	2.3	12
229	Handling Ensemble N-Representability Constraint in Explicit-by-Implicit Manner. Journal of Physical Chemistry Letters, 2021, 12, 6788-6793.	2.1	10
230	The Effect of Hartree-Fock Exchange on Scaling Relations and Reaction Energetics for Câ€“H Activation Catalysts. Topics in Catalysis, 2022, 65, 296-311.	1.3	11
231	Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. Chemical Reviews, 2021, 121, 9927-10000.	23.0	110
232	N-dependent self-interaction corrections: Are they still appealing?. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	0
233	Theoretical study on adiabatic electron affinity of fatty acids. New Journal of Chemistry, 2021, 45, 16892-16905.	1.4	4
234	Proton-transfer dynamics in ionized water chains using real-time time-dependent density functional theory. Physical Review Research, 2020, 2, .	1.3	6
235	Fukui Function. , 2009, , .		37
236	Unity of Kohn-Sham density-functional theory and reduced-density-matrix-functional theory. Physical Review A, 2021, 104, .	1.0	11
237	Exact analytical ground state solution of 1D H$$_2^+$$ with soft Coulomb potential. Journal of Mathematical Chemistry, 2022, 60, 184-194.	0.7	3
238	Study of self-interaction-errors in barrier heights using locally scaled and Perdewâ€“Zunger self-interaction methods. Journal of Chemical Physics, 2022, 156, 014306.	1.2	12

#	Article	IF	Citations
239	Computational Scaling Relationships Predict Experimental Activity and Rate-Limiting Behavior in Homogeneous Water Oxidation. Inorganic Chemistry, 2022, 61, 2186-2197.	1.9	3
240	Eliminating Delocalization Error to Improve Heterogeneous Catalysis Predictions with Molecular DFT + U. Journal of Chemical Theory and Computation, 2022, 18, 1142-1155.	2.3	7
241	Functional-Based Description of Electronic Dynamic and Strong Correlation: Old Issues and New Insights. Journal of Physical Chemistry Letters, 2022, 13, 1744-1751.	2.1	6
242	Approximate functionals in hypercomplex Kohnâ€“Sham theory. Electronic Structure, 2022, 4, 014011.	1.0	3
243	Study of Self-Interaction Errors in Density Functional Calculations of Magnetic Exchange Coupling Constants Using Three Self-Interaction Correction Methods. Journal of Physical Chemistry A, 2022, 126, 1923-1935.	1.1	6
245	Molecular orbital projectors in non-empirical jmDFT recover exact conditions in transition-metal chemistry. Journal of Chemical Physics, 2022, 156, 184112.	1.2	2
246	Ligand Additivity and Divergent Trends in Two Types of Delocalization Errors from Approximate Density Functional Theory. Journal of Physical Chemistry Letters, 2022, 13, 4549-4555.	2.1	2
247	Complex Fermiâ€“LÃ¶wdin orbital self-interaction correction. Journal of Chemical Physics, 2022, 156, .	1.2	5
248	Systematically Improvable Generalization of Self-Interaction Corrected Density Functional Theory. Journal of Physical Chemistry Letters, 2022, 13, 5698-5702.	2.1	5
249	Effects of non-local exchange functionals in the density functional theories for the description of molecular vibrations. Journal of Chemical Sciences, 2022, 134, .	0.7	2
250	Bloch's theorem in orbital-density-dependent functionals: Band structures from Koopmans spectral functionals. Physical Review B, 2022, 106, .	1.1	5
251	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
252	Delocalization error: The greatest outstanding challenge in densityâ€functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	43
253	Molecular interactions from the density functional theory for chemical reactivity: Interaction chemical potential, hardness, and reactivity principles. Frontiers in Chemistry, 0, 10, .	1.8	9
254	Computational Analysis of Structureâ€“Activity Relationships in Highly Active Homogeneous Rutheniumâ^'Based Water Oxidation Catalysts. Catalysts, 2022, 12, 863.	1.6	2
255	Properties of the density functional response kernels and its implications on chemistry. Journal of Chemical Physics, 2022, 157, .	1.2	5
256	Impacts of polarizable continuum models on the SCF convergence and DFT delocalization error of large molecules. Journal of Chemical Physics, 2022, 157, .	1.2	2
257	Electrochemistry from the atomic scale, in the electronically grand-canonical ensemble. Journal of Chemical Physics, 2022, 157, .	1.2	8

#	Article	IF	Citations
258	Mean Value Ensemble Hubbard-U Correction for Spin-Crossover Molecules. Journal of Physical Chemistry Letters, 2022, 13, 12049-12054.	2.1	3
259	Understanding Density-Driven Errors for Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2023, 19, 532-543.	2.3	11
260	Spin-crossover complexes: Self-interaction correction vs density correction. Journal of Chemical Physics, 2023, 158, .	1.2	4
261	Application of a Simple Density-Functional Approximation to Non-identical Fermions in One-dimensional Confinement. Brazilian Journal of Physics, 2023, 53, .	0.7	0
262	Hubbard U through polaronic defect states. Npj Computational Materials, 2022, 8, .	3.5	3
263	Self-consistent implementation of locally scaled self-interaction-correction method. Journal of Chemical Physics, 2023, 158, .	1.2	6
264	How Do Self-Interaction Errors Associated with Stretched Bonds Affect Barrier Height Predictions?. Journal of Physical Chemistry A, 2023, 127, 1750-1759.	1.1	3
265	Insights into the deviation from piecewise linearity in transition metal complexes from supervised machine learning models. Physical Chemistry Chemical Physics, 2023, 25, 8103-8116.	1.3	2