Tight bound and convexity constraint on the exchange-
the low-density limit, and other formal tests of generali

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Citation Report

#	Article	IF	Citations
1	Real-space analysis of the exchange-correlation energy. International Journal of Quantum Chemistry, 1995, 56, 199-210.	1.0	33
2	On the test of different atomic exchange functionals. International Journal of Quantum Chemistry, 1995, 56, 307-316.	1.0	4
3	Nonlocal density functional calculations of the jellium metal surface. International Journal of Quantum Chemistry, 1995, 56, 847-860.	1.0	0
4	Constraints on density functionals imposed by the stability conditions of an inhomogeneous system of charged particles. Solid State Communications, 1995, 95, 323-327.	0.9	0
5	Bounds for the exchange and correlation potentials. Physical Review A, 1995, 51, 2851-2856.	1.0	15
6	Hardness of molecules and the band gap of solids within the Kohn-Sham formalism: A perturbation-scaling approach. Physical Review A, 1995, 52, 4493-4499.	1.0	74
7	Semilocal density functionals for exchange and correlation: Theory and applications. Theoretical and Computational Chemistry, 1995, 2, 29-74.	0.2	13
8	Coordinate Scaling Requirements for Approximating Exchange and Correlation. NATO ASI Series Series B: Physics, 1995, , 11-31.	0.2	10
9	Elementary Concepts in Density Functional Theory. Theoretical and Computational Chemistry, 1996, , 3-24.	0.2	12
10	Generalized gradient approximation for the exchange-correlation hole of a many-electron system. Physical Review B, 1996, 54, 16533-16539.	1.1	5,433
11	Exchange functionals and potentials. Molecular Physics, 1996, 87, 1-36.	0.8	235
12	Generalized gradient approximations to density functional theory: comparison with exact results. Theoretical and Computational Chemistry, 1996, , 295-326.	0.2	34
13	Comparison shopping for a gradient-corrected density functional. International Journal of Quantum Chemistry, 1996, 57, 309-319.	1.0	276
14	Comparison of convetional and hybrid density functional approaches. Cationic hydrides of first-row transition metals as a case study. Chemical Physics Letters, 1996, 249, 290-296.	1.2	44
15	Construction of the adiabatic connection. Chemical Physics Letters, 1996, 263, 499-506.	1.2	164
16	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
17	Convexity and the translational-invariance constraint on the exchange-correlation functional. Physical Review A, 1996, 54, 961-963.	1.0	4
18	Comparison of the Beckeâ^'Leeâ^'Yangâ^'Parr and Beckeâ^'Perdewâ^'Wang Exchange-Correlation Functionals for Geometries of Cyclopentadienylâ^'Transition Metal Complexes. Journal of Physical Chemistry A, 1997, 101, 2502-2508.	1.1	20

#	Article	IF	Citations
19	Interplay between fermion condensation and density-wave instability. JETP Letters, 1997, 65, 253-258.	0.4	23
20	A simple model for calculating the phase diagram of Ti. Journal of Physics Condensed Matter, 1997, 9, L491-L496.	0.7	28
21	Calculation of the Phase Diagram of Zr in a Simple Model. Physica Status Solidi (B): Basic Research, 1997, 201, R9-R10.	0.7	9
22	Additive density functional correlation corrections to single particle theories. International Journal of Quantum Chemistry, 1997, 61, 281-285.	1.0	3
23	On the accuracy of molecular exchange-correlation potentials computed from electron densities. Chemical Physics Letters, 1997, 265, 614-620.	1.2	15
24	Superconductivity in the presence of fermion condensation. JETP Letters, 1998, 68, 527-533.	0.4	10
25	Density functional theory of fermion condensation. Physics Letters, Section A: General, Atomic and Solid State Physics, 1998, 249, 237-241.	0.9	28
26	Implementation and validation of the Lacks-Gordon exchange functional in conventional density functional and adiabatic connection methods. Journal of Computational Chemistry, 1998, 19, 418-429.	1.5	91
27	Density functional. Theory and application to atoms and molecules. Physics Reports, 1998, 298, 1-79.	10.3	151
28	Density functionals for non-relativistic coulomb systems. , 1998, , 8-59.		22
29	A novel form for the exchange-correlation energy functional. Journal of Chemical Physics, 1998, 109, 400-410.	1.2	724
30	Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. Journal of Chemical Physics, 1998, 108, 664-675.	1.2	3,068
31	Gradient-corrected Exchange Potential Functional with the correct asymptotic behaviour. Advances in Quantum Chemistry, 1998, 33, 105-130.	0.4	4
32	Derivation of a Generalized Gradient Approximation: The PW91 Density Functional. , 1998, , 81-111.		163
33	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
34	Recent Developments in the Local-Scaling Transformation Version of Density Functional Theory. Advances in Quantum Chemistry, 1998, , 49-70.	0.4	12
35	A reexamination of exchange energy functionals. Journal of Chemical Physics, 1999, 111, 5656-5667.	1.2	21
36	A new one-parameter progressive Colleâ€“Salvetti-type correlation functional. Journal of Chemical Physics, 1999, 110, 10664-10678.	1.2	276

#	Article	IF	Citations
37	Model of a strongly correlated liquid. Physics Letters, Section A: General, Atomic and Solid State Physics, 1999, 259, 460-465.	0.9	4
38	Toward reliable density functional methods without adjustable parameters: The PBE0 model. Journal of Chemical Physics, 1999, 110, 6158-6170.	1.2	14,178
39	An accurate density functional method for the study of magnetic properties: the PBE0 model. Computational and Theoretical Chemistry, 1999, 493, 145-157.	1.5	168
40	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. , 1999, 75, 889-909.		598
41	Quasiparticle dispersion and lineshape in a strongly correlated liquid with the fermion condensate. Physics Letters, Section A: General, Atomic and Solid State Physics, 2000, 275, 124-130.	0.9	5
42	From Classical Density Functionals to Adiabatic Connection Methods. The State of the Art.. Advances in Quantum Chemistry, 2000, 36, 45-75.	0.4	53
43	Pressure and temperature effects on the Î“, N and L-phonons in zirconium. High Pressure Research, 2000, 17, 385-391.	0.4	6
44	Calculated Nb superconducting transition temperature under hydrostatic pressure. Computational Materials Science, 2000, 17, 202-205.	1.4	12
45	Pressure and temperature effects on the Î“ and N-phonons in zirconium. Computational Materials Science, 2000, 17, 361-364.	1.4	4
46	Calculated Nb superconducting transition temperature under hydrostatic pressure. High Pressure Research, 2000, 17, 393-400.	0.4	3
47	DFT Calculations for Cu-, Ag-, and Au-Containing Molecules. Journal of Physical Chemistry A, 2001, 105, 7905-7916.	1.1	98
48	Quasiparticles in a strongly correlated liquid with the fermion condensate: applications to high-temperature superconductors. Journal of Experimental and Theoretical Physics, 2001, 92, 287-296.	0.2	10
49	Research activities of the theoretical chemistry group at the University of Tokyo. Computational and Theoretical Chemistry, 2001, 573, 91-128.	1.5	13
50	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
51	A transversing connection between density functionals. Journal of Chemical Physics, 2001, 114, 6505-6513.	1.2	19
52	Steric and Electronic Structure of C6H5XCF3 Molecules (X = O or S): A Quantum-Chemical Study. Russian Journal of General Chemistry, 2003, 73, 229-239.	0.3	4
53	Density Functionals for Non-relativistic Coulomb Systems in the New Century. Lecture Notes in Physics, 2003, , 1-55.	0.3	96
54	Assessing the reliability of density functional methods in the conformational study of polypeptides: The treatment of intraresidue nonbonding interactions. Journal of Computational Chemistry, 2004, 25, 1333-1341.	1.5	55

#	Article	IF	Citations
55	From The Cover: The X3LYP extended density functional for accurate descriptions of nonbond interactions, spin states, and thermochemical properties. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 2673-2677.	3.3	863
56	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. Journal of Chemical Physics, 2004, 120, 6898-6911.	1.2	431
57	An extended hybrid density functional (X3LYP) with improved descriptions of nonbond interactions and thermodynamic properties of molecular systems. Journal of Chemical Physics, 2005, 122, 014105.	1.2	204
58	Differential virial theorem in relation to a sum rule for the exchange-correlation force in density-functional theory. Journal of Chemical Physics, 2005, 123, 194104.	1.2	1
59	Progress in the development of exchange-correlation functionals. , 2005, , 669-724.		108
60	Exact energy expression in the strong-interaction limit of the density functional theory. Philosophical Magazine, 2006, 86, 2101-2114.	0.7	2
61	Meta-generalized gradient approximation: non-empirical construction and performance of a density functional. Philosophical Magazine, 2007, 87, 1071-1084.	0.7	11
62	Excited state properties of sizable molecules in solution: from structure to reactivity. Theoretical Chemistry Accounts, 2007, 117, 1073-1084.	0.5	10
63	The excited states of adenine and thymine nucleoside and nucleotide in aqueous solution: a comparative study by time-dependent DFT calculations. Theoretical Chemistry Accounts, 2008, 120, 491-497.	0.5	50
64	Can TDâ€ÐDFT calculations accurately describe the excited states behavior of stacked nucleobases? The cytosine dimer as a test case. Journal of Computational Chemistry, 2008, 29, 957-964.	1.5	59
65	Assessment of density functionals for the investigation of iridium(III) complexes. Computational and Theoretical Chemistry, 2008, 861, 97-102.	1.5	19
66	What can we learn from the adiabatic connection formalism about local hybrid functionals?. Journal of Chemical Physics, 2008, 128, 214107.	1.2	44
68	Lower Bounds on the Exchange-Correlation Energy in Reduced Dimensions. Physical Review Letters, 2009, 102, 206406.	2.9	37
69	Variable Liebâ€“Oxford bound satisfaction in a generalized gradient exchange-correlation functional. Journal of Chemical Physics, 2009, 130, 244103.	1.2	36
70	DFT/TDâ€ÐDFT investigation on Ir(III) complexes with Nâ€heterocyclic carbene ligands: Geometries, electronic structures, absorption, and phosphorescence properties. Journal of Computational Chemistry, 2010, 31, 628-638.	1.5	25
71	Linearized orbitalâ€free embedding potential in selfâ€consistent calculations. International Journal of Quantum Chemistry, 2009, 109, 1886-1897.	1.0	14
72	Role of exchange in density-functional theory for weakly interacting systems: Quantum Monte Carlo analysis of electron density and interaction energy. Physical Review A, 2009, 80, .	1.0	21
73	On the lower bound on the exchange-correlation energy in two dimensions. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 1236-1238.	1.3	0

#	Article	IF	Citations
74	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
75	Hyperfine coupling constants of the nitrogen and phosphorus atoms: A challenge for exact-exchange density-functional and post-Hartreeâ€"Fock methods. Journal of Chemical Physics, 2010, 132, 184107.	1.2	15
77	Double-hybrid density-functional theory made rigorous. Journal of Chemical Physics, 2011, 134, 064113.	1.2	165
78	Rigorous formulation of two-parameter double-hybrid density-functionals. Journal of Chemical Physics, 2011, 135, 244106.	1.2	43
79	Oxidovanadium(IV) Schiff Base Complex Derived from Vitamin B₆: Synthesis, Characterization, and Insulin Enhancing Properties. Inorganic Chemistry, 2011, 50, 4349-4361.	1.9	66
81	Strictly correlated uniform electron droplets. Physical Review B, 2011, 83, .	1.1	29
82	Study of the orbital hardness and the Kohnâ€Sham radius on single monoatomic anions. International Journal of Quantum Chemistry, 2011, 111, 3097-3111.	1.0	3
83	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
84	Indirect Coulomb energy for two-dimensional atoms. Journal of Mathematical Physics, 2012, 53, .	0.5	4
85	Improved constraint satisfaction in a simple generalized gradient approximation exchange functional. Journal of Chemical Physics, 2012, 136, 144115.	1.2	31
86	Optimal-transport formulation of electronic density-functional theory. Physical Review A, 2012, 85, .	1.0	101
87	Performance of Gradient-Corrected and Hybrid Density Functional Theory: Role of the Underlying Local Density Approximation and the Gradient Correction. Journal of Chemical Theory and Computation, 2012, 8, 4899-4906.	2.3	16
88	Violation of a local form of the Lieb-Oxford bound. Physical Review A, 2012, 85, .	1.0	12
89	Tuning electronic structure and photophysical properties of [Ir(ppy)2(py)2]+ by substituents binding in pyridyl ligand: a computational study. Journal of Molecular Modeling, 2012, 18, 4615-4624.	0.8	3
90	Energy Densities in the Strong-Interaction Limit of Density Functional Theory. Journal of Chemical Theory and Computation, 2012, 8, 3097-3107.	2.3	43
91	A new meta-GGA exchange functional based on an improved constraint-based GGA. Chemical Physics Letters, 2012, 543, 179-183.	1.2	44
92	A multiconfigurational hybrid density-functional theory. Journal of Chemical Physics, 2012, 137, 044104.	1.2	77
93	A New Estimate on the Two-Dimensional Indirect Coulomb Energy. Annales Henri Poincare, 2012, 13, 1733-1744.	0.8	8

#	Article	IF	Citations
94	A new estimate on the indirect Coulomb energy. International Journal of Quantum Chemistry, 2012, 112, 1579-1584.	1.0	12
95	Hyper-generalized-gradient functionals constructed from the Lieb-Oxford bound: Implementation via local hybrids and thermochemical assessment. Journal of Chemical Physics, 2012, 136, 184102.	1.2	33
96	Effects of molecular dynamics and solvation on the electronic structure of molecular probes. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	5
97	Computational 17O-NMRspectroscopy of organic acids and peracids: comparison of solvation models. Physical Chemistry Chemical Physics, 2013, 15, 1130-1140.	1.3	8
98	Solvent effect on UV/Vis absorption and emission spectra in aqueous solution based on a modified form of solvent reorganization energy. Chemical Physics Letters, 2013, 583, 213-217.	1.2	10
99	Analysis of double-hybrid density functionals along the adiabatic connection. Molecular Physics, 2013, 111, 1275-1294.	0.8	42
100	Gedanken densities and exact constraints in density functional theory. Journal of Chemical Physics, 2014, 140, 18A533.	1.2	82
101	The excited state behavior of cytosine in the gas phase: A TD-DFT study. Computational and Theoretical Chemistry, 2014, 1040-1041, 186-194.	1.1	25
102	Double-hybrid density-functional theory with meta-generalized-gradient approximations. Journal of Chemical Physics, 2014, 140, 084107.	1.2	35
103	Generalized gradient approximation exchange energy functional with correct asymptotic behavior of the corresponding potential. Journal of Chemical Physics, 2015, 142, 054105.	1.2	42
104	Improved Lieb-Oxford exchange-correlation inequality with a gradient correction. Physical Review A, 2015, 91, .	1.0	35
105	Hydrogen Molecule Dissociation Curve with Functionals Based on the Strictly Correlated Regime. Journal of Chemical Theory and Computation, 2015, 11, 3153-3162.	2.3	31
106	Wave-function inspired density functional applied to the H₂/${{m{H}}}_{2}^{+}$ challenge. New Journal of Physics, 2016, 18, 073026.	1.2	12
107	Unexpected cold curve sensitivity to GGA exchange form. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	0
108	A power series revisit of the PBE exchange density-functional approximation: The PBEpow model. Journal of Chemical Physics, 2016, 145, 244102.	1.2	3
109	A PW91-like exchange with a simple analytical form. Chemical Physics Letters, 2016, 651, 268-273.	1.2	16
110	Challenging the Liebâ€“Oxford bound in a systematic way. Molecular Physics, 2016, 114, 1076-1085.	0.8	22
111	B88 exchange functional recovering the local spin density linear response. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	2

#	Article	IF	Citations
112	Kineticâ€energyâ€density dependent semilocal exchangeâ€correlation functionals. International Journal of Quantum Chemistry, 2016, 116, 1641-1694.	1.0	78
113	Assessing the concept of structure sensitivity or insensitivity for sub-nanometer catalyst materials. Surface Science, 2016, 652, 7-19.	0.8	36
114	Structure sensitivity in the nonscalable regime explored via catalysed ethylene hydrogenation on supported platinum nanoclusters. Nature Communications, 2016, 7, 10389.	5.8	115
115	Gradient-regulated connection-based correction for the PBE exchange: the PBEtrans model. Molecular Physics, 2016, 114, 1059-1065.	0.8	3
116	Density Functional Model for Nondynamic and Strong Correlation. Journal of Chemical Theory and Computation, 2016, 12, 133-143.	2.3	56
117	Theoretical study on electronic excitation spectra: A matrix form of numerical algorithm for spectral shift. Chemical Physics, 2017, 492, 27-34.	0.9	3
118	Simple Fully Nonlocal Density Functionals for Electronic Repulsion Energy. Journal of Physical Chemistry Letters, 2017, 8, 2799-2805.	2.1	30
119	Augmented potential, energy densities, and virial relations in the weak- and strong-interaction limits of DFT. Journal of Chemical Physics, 2017, 147, 214107.	1.2	22
120	Symmetry Breaking in the Periodic Thomasâ€“Fermiâ€“Diracâ€“von WeizsÃcker Model. Annales Henri Poincare, 2018, 19, 3129-3177.	0.8	4
121	Response Potential in the Strong-Interaction Limit of Density Functional Theory: Analysis and Comparison with the Coupling-Constant Average. Journal of Chemical Theory and Computation, 2018, 14, 4151-4167.	2.3	21
122	Novel nonequilibrium solvation theory for calculating the solvatochromic Stokes shift by State-specific TD-DFT. Chemical Physics Letters, 2019, 732, 136640.	1.2	6
123	Coordinate Scaling in Time-Independent Excited-State Density Functional Theory for Coulomb Systems. Computation, 2019, 7, 59.	1.0	2
124	Generalized Gradient Approximation Exchange Energy Functional with Near-Best Semilocal Performance. Journal of Chemical Theory and Computation, 2019, 15, 303-310.	2.3	24
125	The local density approximation in density functional theory. Pure and Applied Analysis, 2020, 2, 35-73.	0.4	23
126	One-dimensional Liebâ€“Oxford bounds. Journal of Chemical Physics, 2020, 152, 234112.	1.2	0
127	A New Mixing of Nonlocal Exchange and Nonlocal Correlation with Multiconfiguration Pair-Density Functional Theory. Journal of Physical Chemistry Letters, 2020, 11, 10158-10163.	2.1	21
128	Generalized gradient approximations with local parameters. Physical Review B, 2020, 102, .	1.1	9
129	Extended Koopmansâ€™ theorem in the adiabatic connection formalism: Applied to doubly hybrid density functionals. Journal of Chemical Physics, 2020, 153, 044109.	1.2	5

#	Article	IF	Citations
130	Analysis of the kinetic energy functional in the generalized gradient approximation. Journal of Chemical Physics, 2021, 154, 084107.	1.2	7
131	Accurate density functional made more versatile. Journal of Chemical Physics, 2021, 155, 024103.	1.2	15
132	Thomas-Fermi and Other Density-Functional Theories. , 2006, , 295-306.		4
133	Density Gradient Expansion of the Electronic Exchange-Correlation Energy, and its Generalization. NATO ASI Series Series B: Physics, 1995, , 51-64.	0.2	3
134	Mixing Exact Exchange with GGA: When to Say When. , 1998, , 57-68.		32
135	On Some Open Problems in Many-Electron Theory. Letters in Mathematical Physics, 2014, , 413-417.	0.4	3
136	A New Generation of Doubly Hybrid Density Functionals (DHDFs). Springer Briefs in Molecular Science, 2014, , 25-45.	0.1	2
137	Can Density Functional Theory Describe Strongly Correlated Electronic Systems?. , 2002, , 237-252.		2
138	The Standard ASW Method. Lecture Notes in Physics, 2012, , 5-44.	0.3	0
139	Effects of molecular dynamics and solvation on the electronic structure of molecular probes. Highlights in Theoretical Chemistry, 2013, , 339-350.	0.0	0
140	An Overview of Modern Density Functional Theory. Springer Briefs in Molecular Science, 2014, , 1-24.	0.1	0
141	Present Status of the First-Principles Electronic Structure Calculations for the Strongly Correlated Transition-Metal Oxides. Springer Series in Solid-state Sciences, 1999, , 34-44.	0.3	0
142	Rearrangement of the Single-Particle Degrees of Freedom. Springer Tracts in Modern Physics, 2020, , 71-87.	0.1	0
143	The Standard ASW Method. , 2007, , 5-45.		0
144	Construction of meta-GGA functionals through restoration of exact constraint adherence to regularized SCAN functionals. Journal of Chemical Physics, 2022, 156, 034109.	1.2	25
145	Laplacian-level meta-generalized gradient approximation for solid and liquid metals. Physical Review Materials, 2022, 6, .	0.9	10
146	DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. Physical Chemistry Chemical Physics, 2022, 24, 28700-28781.	1.3	91
147	Density functionals based on the mathematical structure of the strongâ€interaction limit of <scp>DFT</scp>. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	11

#	Article	IF	Citations
148	Improved Liebâ€“Oxford bound on the indirect and exchange energies. Letters in Mathematical Physics, 2022, 112, .	0.5	9
149	The Predictive Power of Exact Constraints and Appropriate Norms in Density Functional Theory. Annual Review of Physical Chemistry, 2023, 74, 193-218.	4.8	22
150	Thomas-Fermi and Other Density-Functional Theories. Springer Handbooks, 2023, , 297-308.	0.3	0
151	Classical Density Functional Theory: Representability and Universal Bounds. Journal of Statistical Physics, 2023, 190, .	0.5	0
152	Seven useful questions in density functional theory. Letters in Mathematical Physics, 2023, 113, .	0.5	6
153	Review of Approximations for the Exchange-Correlation Energy in Density-Functional Theory. , 2023, , 1-90.		3
154	Universal Functionals in Density Functional Theory. , 2023, , 115-182.		1