

Influential Functionals

M.K. Horton*

Materials Science Division, Lawrence Berkeley National Laboratory

(Dated: November 3, 2022)

Learning about density functional approximations (DFAs), or approximations for the exchange-correlation functional, can be intimidating. Density Functional Theory is now one of the primary simulation tools for the practicing chemist or materials scientist, and its accuracy relies upon an appropriate choice of DFA. Over the past decades, there has been extensive research effort to find better DFAs, and there is now a large body of literature to read through for someone learning about DFAs for the first time. In this brief report, I share an analysis that suggests which functionals and publications have been the most influential, as a potential reading list to new scientists in this area. Here, “influential” is defined as “likely to have informed the design of another functional”, and not simply a measure of number of citations, or how much that functional has been used for practical applications. This analysis is not claimed to be complete.

I. INTRODUCTION

This brief report assumes some prior familiarity with Density Functional Theory and density functional approximations, and specifically of exchange-correlation functionals. It is not intended to be a rigorous work, or to be an alternative to a good literature review (of which there are many!), but simply to list which functionals and publications have been highly influential, so as to provide a reading list for those new to the field.

Here, “influential” refers to how much a functional has somehow informed the design of new functionals, rather than simply how often it has been cited: the latter is good measure of its overall impact, and how much that functional has been used and has been practically beneficial, but does not necessarily capture the importance of the functional for the development of new functionals. Indeed, many pioneering publications in functional development have not seen many citations, since they have not seen much practical usage but were instead stepping stones to the development of more widely-adopted functionals.

The other motivation for writing up this analysis is to demonstrate a somewhat less biased method of performing a literature review through the combination of routine data retrieval and analysis methods.

II. READING LIST

The most influential functionals are listed in Tables I, II, III, and IV for those published before 1990, 1990–2000, 2000–2010, and 2010–present, respectively.

In addition, Table V shows papers that are highly cited by these publications, but which do not themselves

propose a functional of their own; that is, these are important background reading about the DFT method or key concepts therein.

III. METHOD

The `libxc`[1, 2] library is a carefully curated, and well-documented, library of exchange-correlation functionals ready for use in other codes. It is difficult to overstate the achievement that is `libxc` or its value to the community as a resource. For the analysis here, the digital object identifiers (DOIs) of functionals used in `libxc` are collected, and their references obtained via the Crossref API[3].

A directed graph is constructed with each DOI as a node and a citing relationship as an edge. Link ranking algorithms PageRank[4] and HITS[5] are applied. All graph analysis is performed using the `networkx`[6] library.

In the tables, “PR#” refers to the overall Pagerank rank index, “A#” refers to the overall “authorities” rank index, as defined by the HITS algorithm, and “Citations” refers to the total number of citations for that publication.

In total, 398 references are retrieved from the `libxc` library. The resulting graph, including all references of all 398 publications, has 7366 nodes and 20818 edges. At a paper a day, reading all relevant publications would take over two decades, so this author suggests an effort to rank these papers is well-motivated!

There are some caveats with this data. First, it may not be complete, since `libxc` may be missing some functionals. Secondly, information on the references of some publications were not available via Crossref, and were omitted from the analysis. Finally, some references required additional Crossref queries to obtain a DOI, and this process can provide an incorrect DOI in some instances. While this means that some important pub-

* Email address: mkhorton@lbl.gov

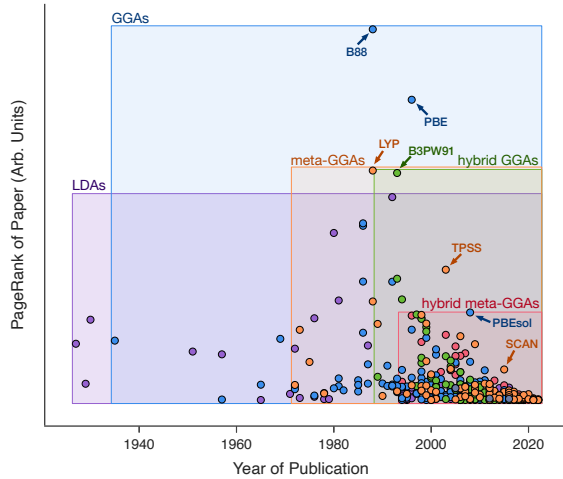


Figure 1. A graph of the PageRank of a given publication (a proxy for its influence), against year of publication. Shaded regions show when specific types of functional were introduced.

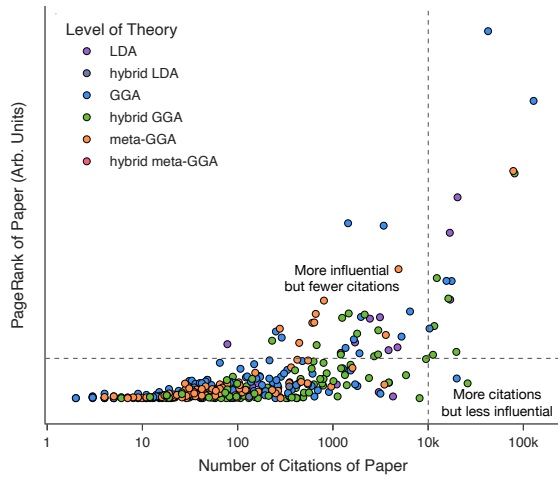


Figure 2. A graph of the PageRank of a given publication (a proxy for its influence) against its overall number of citations.

lications have been omitted, these caveats are not expected to significantly change the overall ranking of those publications that have been included.

IV. DATA AVAILABILITY STATEMENT

Data has been uploaded to MPContribs and is available at https://contribs.materialsproject.org/projects/influential_functionals.

AUTHOR'S NOTE

This brief report originated purely from personal curiosity and was written up for fun. It is only shared since it may be of some legitimate interest to the community, but with the understanding that this is only a quick, preliminary analysis and this report has not been peer-reviewed. I would be grateful to accept corrections for revision. This paper and analysis are shared under CC-BY, so if it's useful for someone to reuse, please do so.

- [1] M. A. Marques, M. J. Oliveira, and T. Burnus, *Computer physics communications* **183**, 2272 (2012).
- [2] S. Lehtola, C. Steigemann, M. J. Oliveira, and M. A. Marques, *SoftwareX* **7**, 1 (2018).
- [3] Crossref, "REST API," <https://www.crossref.org/documentation/retrieve-metadata/rest-api/>.
- [4] L. Page, S. Brin, R. Motwani, and T. Winograd, *The PageRank citation ranking: Bringing order to the web.*, Tech. Rep. (Stanford InfoLab, 1999).

- [5] J. M. Kleinberg, *Journal of the ACM (JACM)* **46**, 604 (1999).
- [6] A. Hagberg, P. Swart, and D. S. Chult, *Exploring network structure, dynamics, and function using NetworkX*, Tech. Rep. (Los Alamos National Lab.(LANL), Los Alamos, NM (United States), 2008).

Table I. Influential functionals from before 1990.

PR#	AR#	Citations	Label	Theory	Citation
1	2	42576	B88	GGA	Becke, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior. <i>Physical Review A</i> 38, 3098–3100 (1988).
4	4	78367	LYP, HFLYP, CS	meta-GGA	Lee, C., Yang, W. & Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. <i>Physical Review B</i> 37, 785–789 (1988).
9	53	1443	B86	GGA	Becke, A. D. Density functional calculations of molecular bond energies. <i>The Journal of Chemical Physics</i> 84, 4524–4529 (1986).
10	21	3411	PW86	GGA	Perdew, J. P. & Yue, W. Accurate and simple density functional for the electronic exchange energy: Generalized gradient approximation. <i>Physical Review B</i> 33, 8800–8802 (1986).
11	10	16880	VWN	LDA	Vosko, S. H., Wilk, L. & Nusair, M. Accurate spin-dependent electron liquid correlation energies for local spin density calculations: a critical analysis. <i>Canadian Journal of Physics</i> 58, 1200–1211 (1980).
16	37	15571	P86	GGA	Perdew, J. P. Density-functional approximation for the correlation energy of the inhomogeneous electron gas. <i>Physical Review B</i> 33, 8822–8824 (1986).
26	27	17052	PZ	LDA	Perdew, J. P. & Zunger, A. Self-interaction correction to density-functional approximations for many-electron systems. <i>Physical Review B</i> 23, 5048–5079 (1981).
27	121	805	B88	meta-GGA	Becke, A. D. Correlation energy of an inhomogeneous electron gas: A coordinate-space model. <i>The Journal of Chemical Physics</i> 88, 1053–1062 (1988).
34	76	3119	GL	LDA	Gunnarsson, O. & Lundqvist, B. I. Exchange and correlation in atoms, molecules, and solids by the spin-density-functional formalism. <i>Physical Review B</i> 13, 4274–4298 (1976).
36	89	2447	-	LDA	Dirac, P. A. M. Note on Exchange Phenomena in the Thomas Atom. <i>Mathematical Proceedings of the Cambridge Philosophical Society</i> 26, 376–385 (1930).
39	57	608	BR89	meta-GGA	Becke, A. D. & Roussel, M. R. Exchange holes in inhomogeneous systems: A coordinate-space model. <i>Physical Review A</i> 39, 3761–3767 (1989).
45	382	277	GEA4	meta-GGA	Hodges, C. H. Quantum Corrections to the Thomas–Fermi Approximation—The Kirzhnits Method. <i>Canadian Journal of Physics</i> 51, 1428–1437 (1973).
48	227	252	B86_MGC, B86_R	GGA	Becke, A. D. On the large-gradient behavior of the density functional exchange energy. <i>The Journal of Chemical Physics</i> 85, 7184–7187 (1986).
55	466	290	HERMAN	GGA	Herman, F., Van Dyke, J. P. & Ortenburger, I. B. Improved Statistical Exchange Approximation for Inhomogeneous Many-Electron Systems. <i>Physical Review Letters</i> 22, 807–811 (1969).
57	133	1660	TFVW, VW	GGA	Weizsäcker, C. F. v. Zur Theorie der Kernmassen. <i>Zeitschrift für Physik</i> 96, 431–458 (1935).

Table II. Influential functionals from between 1990 and 2000.

PR#	AR#	Citations	Label	Theory	Citation
3	1	127934	PBE	GGA	Perdew, J. P., Burke, K. & Ernzerhof, M. Generalized Gradient Approximation Made Simple. <i>Physical Review Letters</i> 77, 3865–3868 (1996).
5	5	80876	B3PW91	hybrid GGA	Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. <i>The Journal of Chemical Physics</i> 98, 5648–5652 (1993).
6	7	20350	PW	LDA	Perdew, J. P. & Wang, Y. Accurate and simple analytic representation of the electron-gas correlation energy. <i>Physical Review B</i> 45, 13244–13249 (1992).
15	16	12327	BHANDH, BHANDHLYP	hybrid GGA	Becke, A. D. A new mixing of Hartree–Fock and local density-functional theories. <i>The Journal of Chemical Physics</i> 98, 1372–1377 (1993).
17	36	17648	PW91	GGA	Perdew, J. P. et al. Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. <i>Physical Review B</i> 46, 6671–6687 (1992).
25	8	16292	B3LYP	hybrid GGA	Stephens, P. J., Devlin, F. J., Chabalowski, C. F. & Frisch, M. J. Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields. <i>The Journal of Physical Chemistry</i> 98, 11623–11627 (1994).
30	22	1465	B97	hybrid GGA	Becke, A. D. Density-functional thermochemistry. V. Systematic optimization of exchange-correlation functionals. <i>The Journal of Chemical Physics</i> 107, 8554–8560 (1997).
31	11	660	GVT4, VSXC	meta-GGA	Van Voorhis, T. & Scuseria, G. E. A novel form for the exchange-correlation energy functional. <i>The Journal of Chemical Physics</i> 109, 400–410 (1998).
32	20	2155	BC95, B86B95, ...	hybrid meta-GGA	Becke, A. D. Density-functional thermochemistry. IV. A new dynamical correlation functional and implications for exact-exchange mixing. <i>The Journal of Chemical Physics</i> 104, 1040–1046 (1996).
33	42	1970	PBE_R	GGA	Zhang, Y. & Yang, W. Comment on “Generalized Gradient Approximation Made Simple”. <i>Physical Review Letters</i> 80, 890–890 (1998).
35	17	1251	HCTH_A, ...	hybrid GGA	Hamprecht, F. A., Cohen, A. J., Tozer, D. J. & Handy, N. C. Development and assessment of new exchange-correlation functionals. <i>The Journal of Chemical Physics</i> 109, 6264–6271 (1998).
38	28	637	PKZB	meta-GGA	Perdew, J. P., Kurth, S., Zupan, A. & Blaha, P. Accurate Density Functional with Correct Formal Properties: A Step Beyond the Generalized Gradient Approximation. <i>Physical Review Letters</i> 82, 2544–2547 (1999).
40	13	11608	PBEH	hybrid GGA	Adamo, C. & Barone, V. Toward reliable density functional methods without adjustable parameters: The PBE0 model. <i>The Journal of Chemical Physics</i> 110, 6158–6170 (1999).
44	70	10347	PBE	GGA	Perdew, J. P., Burke, K. & Ernzerhof, M. Generalized Gradient Approximation Made Simple [Phys. Rev. Lett. 77, 3865 (1996)]. <i>Physical Review Letters</i> 78, 1396–1396 (1997).
46	41	2996	PBEH	hybrid GGA	Ernzerhof, M. & Scuseria, G. E. Assessment of the Perdew–Burke–Ernzerhof exchange-correlation functional. <i>The Journal of Chemical Physics</i> 110, 5029–5036 (1999).

Table III. Influential functionals from between 2000 and 2010.

PR#	AR#	Citations	Label	Theory	Citation
12	6	4884	TPSS	meta-GGA	Tao, J., Perdew, J. P., Staroverov, V. N. & Scuseria, G. E. Climbing the Density Functional Ladder: Nonempirical Meta-Generalized Gradient Approximation Designed for Molecules and Solids. <i>Physical Review Letters</i> 91, (2003).
29	12	6452	PBE_SOL	GGA	Perdew, J. P. et al. Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces. <i>Physical Review Letters</i> 100, (2008).
50	14	1797	TPSSH	hybrid meta-GGA	Staroverov, V. N., Scuseria, G. E., Tao, J. & Perdew, J. P. Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. <i>The Journal of Chemical Physics</i> 119, 12129–12137 (2003).
52	9	3595	M06_L	meta-GGA	Zhao, Y. & Truhlar, D. G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. <i>The Journal of Chemical Physics</i> 125, 194101 (2006).
63	26	443	REGTPSS, REVTPSS	meta-GGA	Perdew, J. P., Ruzsinszky, A., Csonka, G. I., Constantin, L. A. & Sun, J. Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. <i>Physical Review Letters</i> 103, (2009).
68	15	675	MPW1KCIS, MPWKCIS1K	hybrid meta-GGA	Zhao, Y., González-García, N. & Truhlar, D. G. Benchmark Database of Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions and Its Use to Test Theoretical Methods. <i>The Journal of Physical Chemistry A</i> 109, 2012–2018 (2005).
72	34	1357	ITYH_OPTX, OPTX	GGA	Handy, N. C. & Cohen, A. J. Left-right correlation energy. <i>Molecular Physics</i> 99, 403–412 (2001).
79	29	19784	M06, M06_2X, ...	hybrid meta-GGA	Zhao, Y. & Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. <i>Theoretical Chemistry Accounts</i> 120, 215–241 (2007).
81	61	1901	ITYH, ...	GGA	Iikura, H., Tsuneda, T., Yanai, T. & Hirao, K. A long-range correction scheme for generalized-gradient-approximation exchange functionals. <i>The Journal of Chemical Physics</i> 115, 3540–3544 (2001).
84	25	2981	M05_2X	hybrid meta-GGA	Zhao, Y., Schultz, N. E. & Truhlar, D. G. Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> 2, 364–382 (2006).
85	32	1211	PW6B95, PWB6K	hybrid meta-GGA	Zhao, Y. & Truhlar, D. G. Design of Density Functionals That Are Broadly Accurate for Thermochemistry, Thermochemical Kinetics, and Nonbonded Interactions. <i>The Journal of Physical Chemistry A</i> 109, 5656–5667 (2005).
86	54	11244	HSE03	hybrid GGA	Heyd, J., Scuseria, G. E. & Ernzerhof, M. Hybrid functionals based on a screened Coulomb potential. <i>The Journal of Chemical Physics</i> 118, 8207–8215 (2003).
95	56	9496	CAM_B3LYP	hybrid GGA	Yanai, T., Tew, D. P. & Handy, N. C. A new hybrid exchange–correlation functional using the Coulomb-attenuating method (CAM-B3LYP). <i>Chemical Physics Letters</i> 393, 51–57 (2004).
99	59	216	SOGGA	GGA	Zhao, Y. & Truhlar, D. G. Construction of a generalized gradient approximation by restoring the density-gradient expansion and enforcing a tight Lieb–Oxford bound. <i>The Journal of Chemical Physics</i> 128, 184109 (2008).
101	63	478	AM05	GGA	Armiento, R. & Mattsson, A. E. Functional designed to include surface effects in self-consistent density functional theory. <i>Physical Review B</i> 72, (2005).

Table IV. Influential functionals from after 2010.

PR#	AR#	Citations	Label	Theory	Citation
130	64	1604	SCAN	meta-GGA	Sun, J., Ruzsinszky, A. & Perdew, J. P. Strongly Constrained and Appropriately Normed Semilocal Density Functional. <i>Physical Review Letters</i> 115, (2015).
137	86	107	APBE, VAPBE	RE- GGA	Constantin, L. A., Fabiano, E., Laricchia, S. & Della Sala, F. Semiclassical Neutral Atom as a Reference System in Density Functional Theory. <i>Physical Review Letters</i> 106, (2011).
229	107	157	SOGGA11	GGA	Peeverati, R., Zhao, Y. & Truhlar, D. G. Generalized Gradient Approximation That Recovers the Second-Order Density-Gradient Expansion with Optimized Across-the-Board Performance. <i>The Journal of Physical Chemistry Letters</i> 2, 1991–1997 (2011).
234	101	142	MS1, MS2_REV, MS2H	MS2, hybrid meta-GGA	Sun, J. et al. Semilocal and hybrid meta-generalized gradient approximations based on the understanding of the kinetic-energy-density dependence. <i>The Journal of Chemical Physics</i> 138, 044113 (2013).
239	88	736	M11	hybrid meta-GGA	Peeverati, R. & Truhlar, D. G. Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. <i>The Journal of Physical Chemistry Letters</i> 2, 2810–2817 (2011).
256	190	48	PBEINT	GGA	Fabiano, E., Constantin, L. A. & Della Sala, F. Generalized gradient approximation bridging the rapidly and slowly varying density regimes: A PBE-like functional for hybrid interfaces. <i>Physical Review B</i> 82, (2010).
293	97	464	M11_L	meta-GGA	Peeverati, R. & Truhlar, D. G. M11-L: A Local Density Functional That Provides Improved Accuracy for Electronic Structure Calculations in Chemistry and Physics. <i>The Journal of Physical Chemistry Letters</i> 3, 117–124 (2011).
303	131	103	MS0	meta-GGA	Sun, J., Xiao, B. & Ruzsinszky, A. Communication: Effect of the orbital-overlap dependence in the meta generalized gradient approximation. <i>The Journal of Chemical Physics</i> 137, 051101 (2012).
308	112	235	N12	GGA	Peeverati, R. & Truhlar, D. G. Exchange–Correlation Functional with Good Accuracy for Both Structural and Energetic Properties while Depending Only on the Density and Its Gradient. <i>Journal of Chemical Theory and Computation</i> 8, 2310–2319 (2012).
336	127	25964	PBE38	hybrid GGA	Grimme, S., Antony, J., Ehrlich, S. & Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H–Pu. <i>The Journal of Chemical Physics</i> 132, 154104 (2010).
344	146	99	MVS, MVSH	hybrid meta-GGA	Sun, J., Perdew, J. P. & Ruzsinszky, A. Semilocal density functional obeying a strongly tightened bound for exchange. <i>Proceedings of the National Academy of Sciences</i> 112, 685–689 (2015).
387	164	53	Q2D	GGA	Chiodo, L., Constantin, L. A., Fabiano, E. & Della Sala, F. Nonuniform Scaling Applied to Surface Energies of Transition Metals. <i>Physical Review Letters</i> 108, (2012).
418	149	790	VV10, LC_VV10	hybrid GGA	Vydrov, O. A. & Van Voorhis, T. Nonlocal van der Waals density functional: The simpler the better. <i>The Journal of Chemical Physics</i> 133, 244103 (2010).
428	2854	32	CHACHIYO, CHACHIYO_MOD	LDA	Chachiyo, T. Communication: Simple and accurate uniform electron gas correlation energy for the full range of densities. <i>The Journal of Chemical Physics</i> 145, 021101 (2016).
436	209	30	VMT84_GE, VMT84_PBE	GGA	Vela, A., Pacheco-Kato, J. C., Gázquez, J. L., del Campo, J. M. & Trickey, S. B. Improved constraint satisfaction in a simple generalized gradient approximation exchange functional. <i>The Journal of Chemical Physics</i> 136, 144115 (2012).

Table V. Influential publications without associated functionals in `libxc`.

PR#	AR#	Citations	Citation
2	3	45996	Kohn, W. & Sham, L. J. Self-Consistent Equations Including Exchange and Correlation Effects. <i>Physical Review</i> 140, A1133–A1138 (1965).
7	104	5227	Clementi, E. & Roetti, C. Roothaan-Hartree-Fock atomic wavefunctions. <i>Atomic Data and Nuclear Data Tables</i> 14, 177–478 (1974).
8	19	38547	Hohenberg, P. & Kohn, W. Inhomogeneous Electron Gas. <i>Physical Review</i> 136, B864–B871 (1964).
13	33	3077	Curtiss, L. A., Raghavachari, K., Trucks, G. W. & Pople, J. A. Gaussian-2 theory for molecular energies of first- and second-row compounds. <i>The Journal of Chemical Physics</i> 94, 7221–7230 (1991).
14	58	780	Levy, M. & Perdew, J. P. Hellmann-Feynman, virial, and scaling requisites for the exact universal density functionals. Shape of the correlation potential and diamagnetic susceptibility for atoms. <i>Physical Review A</i> 32, 2010–2021 (1985).
18	67	937	Langreth, D. C. & Mehl, M. J. Beyond the local-density approximation in calculations of ground-state electronic properties. <i>Physical Review B</i> 28, 1809–1834 (1983).
19	18	1768	Curtiss, L. A., Raghavachari, K., Redfern, P. C. & Pople, J. A. Assessment of Gaussian-2 and density functional theories for the computation of enthalpies of formation. <i>The Journal of Chemical Physics</i> 106, 1063–1079 (1997).
20	179	402	Perdew, J. P. Accurate Density Functional for the Energy: Real-Space Cutoff of the Gradient Expansion for the Exchange Hole. <i>Physical Review Letters</i> 55, 1665–1668 (1985).
21	40	122	Parr, R. G. & Weitao, Y. Density-Functional Theory of Atoms and Molecules. (1995) doi:10.1093/oso/9780195092769.001.0001.
22	105	181	Becke, A. D. Hartree-Fock exchange energy of an inhomogeneous electron gas. <i>International Journal of Quantum Chemistry</i> 23, 1915–1922 (1983).
23	69	12053	Ceperley, D. M. & Alder, B. J. Ground State of the Electron Gas by a Stochastic Method. <i>Physical Review Letters</i> 45, 566–569 (1980).
24	24	382	Lieb, E. H. & Oxford, S. Improved lower bound on the indirect Coulomb energy. <i>International Journal of Quantum Chemistry</i> 19, 427–439 (1981).
28	23	463	Chakravorty, S. J., Gwaltney, S. R., Davidson, E. R., Parpia, F. A. & p Fischer, C. F. Ground-state correlation energies for atomic ions with 3 to 18 electrons. <i>Physical Review A</i> 47, 3649–3670 (1993).
37	110	1283	Pople, J. A., Head-Gordon, M., Fox, D. J., Raghavachari, K. & Curtiss, L. A. Gaussian-1 theory: A general procedure for prediction of molecular energies. <i>The Journal of Chemical Physics</i> 90, 5622–5629 (1989).
41	111	175	Oliver, G. L. & Perdew, J. P. Spin-density gradient expansion for the kinetic energy. <i>Physical Review A</i> 20, 397–403 (1979).
42	483	2080	Becke, A. D. Density-functional thermochemistry. I. The effect of the exchange-only gradient correction. <i>The Journal of Chemical Physics</i> 96, 2155–2160 (1992).
43	39	4057	Perdew, J. P., Ernzerhof, M. & Burke, K. Rationale for mixing exact exchange with density functional approximations. <i>The Journal of Chemical Physics</i> 105, 9982–9985 (1996).
47	30	267	Lynch, B. J. & Truhlar, D. G. Small Representative Benchmarks for Thermochemical Calculations. <i>The Journal of Physical Chemistry A</i> 107, 8996–8999 (2003).
49	6647	2267	Mahan, G. D. Many-Particle Physics. (2000) doi:10.1007/978-1-4757-5714-9.
51	800	31	Sham, L. J. Approximations of the Exchange and Correlation Potentials. <i>Computational Methods in Band Theory</i> 458–468 (1971) doi:10.1007/978-1-4684-1890-3_36.