

REPORT

THEORETICAL CHEMISTRY

Density functional theory is straying from the path toward the exact functional

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The theorems at the core of density functional theory (DFT) state that the energy of a many-electron system in its ground state is fully defined by its electron density distribution. This connection is made via the exact functional for the energy, which minimizes at the exact density. For years, DFT development focused on energies, implicitly assuming that functionals producing better energies become better approximations of the exact functional. We examined the other side of the coin: the energy-minimizing electron densities for atomic species, as produced by 128 historical and modern DFT functionals. We found that these densities became closer to the exact ones, reflecting theoretical advances, until the early 2000s, when this trend was reversed by unconstrained functionals sacrificing physical rigor for the flexibility of empirical fitting.

Density functional theory (DFT) is indispensable for modern quantum-chemical modeling of materials and molecules (1). At its theoretical core are the Hohenberg-Kohn theorems (2), which show that all ground-state properties of a many-electron system are uniquely determined by that system's electron density distribution function over space. There exists an exact functional that yields the exact energy of a system from its exact density. Minimization of this functional at a fixed electron number and a fixed external potential yields the exact electron density and energy, but at an unbearable computational cost (3). Modern DFT

relies on approximations of the exact functional (specifically its exchange-correlation term), which tend to provide an excellent cost/accuracy ratio and are believed to be improving in overall accuracy (4, 5). Most of them were constructed empirically; the coefficients in the corresponding formulas were chosen so that energy differences for some chosen systems were as close to known targets as possible. This approach, however, overlooks the fact that the reproduction of exact energy is not a feature of the exact functional, unless the input electron density is exact as well. Hence, pure energy fitting does not necessarily lead toward the exact functional, nor does good

performance of a functional in energetic tests reflect its closeness to the exact functional. Rather, such fidelity requires the approximate functional to produce both energies and electron densities close to the exact ones. Although it was implicitly assumed that functionals improve along with their energies, this assumption was never tested directly.

An alternative, frequently nonempirical, approach to functional design is based on constraint satisfaction—that is, obeying the known features of the exact functional. However, this method also cannot guarantee closeness to the exact functional, because the number of known exact constraints is severely limited. Peverati and Truhlar (4) in particular argued that known exact constraints can be neglected for the sake of greater flexibility in the energy fitting.

Here, we compared the electron density distributions produced by 128 available functionals with the correct ones [as produced by all-electron coupled cluster singles and doubles (CCSD-full) calculations, which provide nearly exact electron densities for the systems studied]. The historical and methodological trends revealed by this study may provide a helpful viewpoint on density functional development.

To our knowledge, correct reproduction of exact electron density has rarely been a parameterization target during the development of currently available functionals. There was an unsuccessful attempt to use molecular electron densities for reparameterization of a three-parameter hybrid

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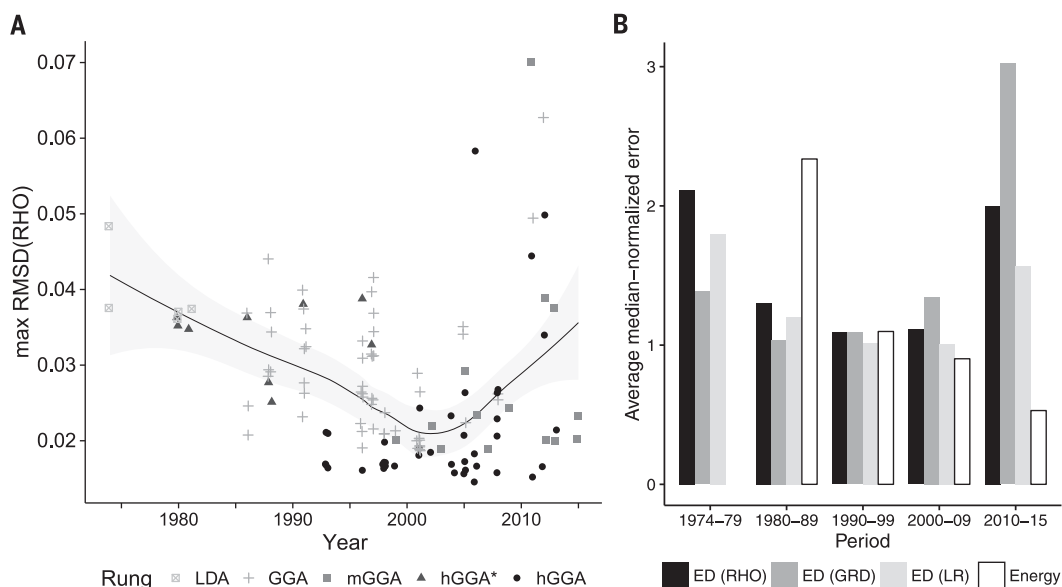


Fig. 1. The historical trends in maximal deviation of the density produced by various DFT methods from the exact one. (A) The line shows the average deviation, with the light gray area denoting its 95% confidence interval; hGGA* denotes 100% exact exchange-based methods. (B) The bars denote averages of DFT functionals' median-normalized absolute error for energy [open bars, Truhlar's data (4)] and electron density with its derivatives (solid bars, this work) per publication decade.

B3LYP (6); Csonka *et al.* also demonstrated (7) that the electron density along the bond in H_2 can be reproduced with high precision by reparameterization of B3P86. The HCTH407 (8) and B97-2 (9) functionals were fitted to reproduce the profile of nearly exact exchange-correlation potentials (and thereby densities) of some atomic and molecular systems. Electron densities produced by several DFT functionals have already been tested in various studies [(10–15) and references therein], but modern highly parameterized functionals were not included.

An attempt to make a fair comparison of densities produced by DFT functionals imposes severe constraints on the systems available for study. The results for molecules would be ambiguous because for typical approximate functionals, accurate molecular energies and densities arise only from an understood but uncontrollable error cancellation between a functional's exchange and correlation components (5). Atoms, however, have been identified as “appropriate norms” (5) for which the exchange and correlation components can be separately accurate. Failure to describe atoms correctly indicates internal problems of a calculation method, which can be expected to propagate to larger systems.

Therefore, we compared calculation results for isolated atoms and atomic cations with 2, 4, or 10 electrons: Be^0 , B^{3+} , B^+ , C^{4+} , C^{2+} , N^{5+} , N^{3+} , O^{6+} , O^{4+} , F^{7+} , F^{5+} , Ne^{8+} , Ne^{6+} , and Ne^0 . All these systems have nondegenerate ground states, so high-level single-reference methods such as CCSD-full provide a standard of accuracy (12). Anions were not included, because semilocal functionals can only bind a fraction of an electron to any neutral atom. Thus, the errors in the densities of anions would reflect not only the functional but also the basis set, and would not fairly measure the relative performances of functionals.

We considered the performance of 128 DFT functionals, including most available from Gaussian09 D.01 (16) and GAMESS-US 20130501R1 (17) codes as separate keywords. In addition, all combinations of pure exchange with pure correlation functionals in GAMESS, as well as several notable literature methods available by adjusting functional parameters in Gaussian, were considered. Modern meta-GGAs—MS0, MS1, MS2, MVS, and SCAN—developed by some of us (18) were also included in the comparison. The tested functionals correspond to the local density approximation (LDA), the generalized gradient approximation (GGA), meta-GGA (mGGA), and hybrid (hGGA) rungs (19). See the supplementary materials for a full list with appropriate citations and reasoning.

To compare DFT with wave function–based methods, we included Hartree-Fock (HF) and Møller-Plesset perturbation [MP2-full, MP3-full, and MP4(sdq)-full] in the comparison. For brevity, we omit the “-full” suffix for post-HF methods.

The exact functional (unlike its inconsistent approximations) should perform better with increasing basis set size, so we have used a quintuple- ζ all-electron aug-cc-pwCV5Z (20) basis set for all calculations. It is augmented with a set of diffuse functions (aug-) for accurate description of outer

electron density and a set of tight functions (ω C) for recovering core and core-valence correlation.

To compare the density distributions between different methods, we used the local electron density (RHO) and two other electron density–based descriptors often used as inputs for DFT functionals: gradient norm of RHO (GRD) and Laplacian of RHO (LR). The deviation of a given descriptor from the CCSD result was calculated as the root mean square difference (RMSD) between the corresponding radial distribution functions. (See difference plots for Ne and Be in figs. S1 to S3.)

The historical trends are obvious from the examination of the RMSD values (for RHO in Fig. 1A; see fig. S4 for all descriptors) over years and for different DFT theory levels. The early LDA methods are surpassed by GGAs, and a marked improvement can be seen with inclusion of Becke's hybrid functional theory, whereas less computationally intensive nonempirical meta-GGAs show performance comparable to that of hGGAs. However, some of the more recent functionals start producing less accurate electron densities than LDAs produce.

To put the errors in RHO, GRD, and LR on the same scale, we divided them by the median RMSD error for each descriptor (one global value per descriptor; see supplementary materials). These median-normalized absolute errors (henceforth

“normalized errors”) are used in all comparisons hereafter. A historical overview of relative DFT performance for electron density descriptors is shown in Fig. 1B and table S1; here, normalized errors are averaged over all functionals and atoms for a given time period. Truhlar's results (4) for energetics are also plotted for comparison using a similar normalization procedure.

The comparison over all descriptors confirms the results seen on individual plots: In recent years, DFT functionals on average are indeed shifting away from the exact functional. To study this unexpected change, a comparison of all three descriptors is necessary. Our set of atoms and ions is not balanced for representation of general quantum-chemical calculations. However, the studied systems can be considered important edge cases: A functional failing at any of these tasks likely has internal problems that will affect the method's performance for other atoms and molecules. We also need to distinguish between methods that fail for one or two particular atoms and those that consistently underperform.

Following this logic, the best methods (L1, Table 1) should have acceptable worst-case behavior and also work well on average. We consider these conditions to be met by functionals residing both (i) in the top quarter of a list

Table 1. The L1 methods (yielding the best densities), their rungs, years, and normalized errors (NE).

Method	Rung	Year	Max NE
CCSD	Ab initio		0.000
MP4sdq	Ab initio		0.246
MP3	Ab initio		0.967
MP2	Ab initio		1.514
mPW3PBE	hGGA	1998	1.778
APFD	hGGA	2012	1.813
B3PW91	hGGA	1993	1.816
PBE0	hGGA	1999	1.818
B98	hGGA	1998	1.826
BHhLYP	hGGA	1993	1.851
B97-3	hGGA	2005	1.883
mPW1PBE	hGGA	1998	1.910
B3P86	hGGA	1993	1.937
O3LYP	hGGA	2001	1.947
PBE1KCIS	hGGA	2005	1.954
mPW1PW91	hGGA	1998	1.955
B97-1	hGGA	1998	1.962
HSE06	hGGA	2006	1.982
PBEh1PBE	hGGA	1998	1.983
B97-2	hGGA	2001	2.018
BlB95	hGGA	1996	2.033
TPSS	mGGA	2003	2.042
TPSSH	hGGA	2003	2.045
TPSSm	mGGA	2007	2.077
X3LYP	hGGA	2005	2.084
SCAN	mGGA	2015	2.107
B3LYP	hGGA	1993	2.123

Table 2. The L2 methods (yielding the worst densities), their rungs, years, and normalized errors (NE).

Method	Rung	Year	Max NE
$X\alpha^*$	LDA	1974	3.777
SP86	GGA	1986	3.821
M06-L	mGGA	2006	3.974
SVWNIRPA	LDA	1980	3.977
SPBE	GGA	1997	3.978
SVWN	LDA	1980	3.984
SPZ81	LDA	1981	3.985
SPW91	GGA	1991	3.989
M06-2X	hGGA	2006	4.027
SOP	GGA	1997	4.182
SLYP	GGA	1988	4.429
M08-SO	hGGA	2008	4.676
SLATER*	LDA	1974	4.864
M08-HX	hGGA	2008	4.880
SOGGA11	GGA	2011	4.971
M06	hGGA	2006	5.420
M06-HF	hGGA	2006	6.125
N12	GGA	2012	6.709
N12-SX	hGGA	2012	6.970
M05	hGGA	2005	7.652
MN12-L	mGGA	2012	8.995
M11	hGGA	2011	10.191
MN12-SX	hGGA	2012	13.005
M11-L	mGGA	2011	15.316

* $\alpha = 0.7$ for $X\alpha$ and $\alpha = 2/3$ for SLATER (see supplementary materials for references).

ordered by the maximum normalized error over individual atoms and descriptors and (ii) in the top quarter of a list ordered by the maximum normalized error over descriptors after averaging over all atoms. A similar definition was used to find the worst-performing functionals (L2, Table 2) residing in the bottom quarter in both lists simultaneously. The studied functionals demonstrate the largest errors in Ne and Ne^{6+} , but the ranking in the tables remains mostly unchanged upon removal of Ne-based systems from the comparison (see supplementary materials for details). Full tables of normalized errors are available in the supplementary materials. Another way to ensure the fairness of the ordering is to average the normalized errors over all descriptors and atoms for a given number of electrons ($n_e = 2, 4, \text{ or } 10$). The resulting table, sorted by maximum error among these three classes, is available in the supplementary materials; its top is populated by L1 functionals and its bottom by L2 ones, with L2 methods showing the worst performance for every n_e .

Two conclusions are immediately apparent. First, functionals constructed with little or no empiricism tend to produce more accurate electron densities than highly empirical ones. Second, at the level of little or no empiricism, the accuracy of the density tends to increase along with the complexity of the density functional approximation as we ascend the Jacob's Ladder (a hierarchy of approximate functionals classified by their inputs) from LDA to GGA to meta-GGA to hybrids (19).

The list of best methods (Table 1) includes four post-HF methods, 20 hybrid functionals, and three meta-GGAs. No DFT functional outperformed the MP2 method. The best hybrid functionals are mainly three- or one-parameter, as proposed by Becke (21, 22). They often include PBE, mPW, or B88 exchange along with PBE, PW91, or LYP correlation. All the best meta-GGAs (TPSS, TPSSm, and SCAN) are the result of thorough constraint-satisfaction work (5, 18, 23, 24). They demonstrate that good accuracy for electron densities (at least for atoms and atomic ions) can be achieved within the meta-GGA form, as can accurate energetics (5, 18, 23, 24).

Hybrid functionals with 100% exact exchange are formally hGGAs but differ in that their exchange and correlation components are strongly misbalanced, so we denote them as hGGA*s. They excellently reproduce LR and are able to describe the two-electron ions relatively well. However, they expectedly fail for systems with higher correlation contribution.

Three functionals (HCTH407, MOHLYP, and revB3LYP) demonstrated good if uneven performance: Their maximum normalized errors for RHO were relatively large (>2.1), whereas the GRD and LR ones were among the lowest for studied functionals. If we were to average the maximum errors over descriptors, these methods would appear among the best, which is notable because MOHLYP and HCTH407 are GGAs.

In the second list (L2, Table 2), the functionals published before 1985 (including all tested LDAs)

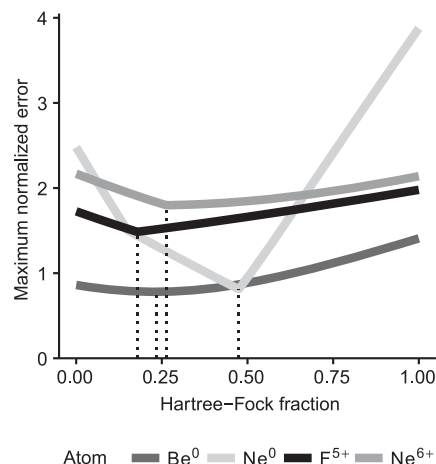


Fig. 2 The maximum normalized errors, $\max(\text{RHO}, \text{GRD}, \text{LR})$, in electron densities produced by the PBE0 functional with the fraction of HF exchange varying from 0 to 1 in increments of 0.05. Solid lines were obtained by spline fitting of the corresponding descriptors. Minima are denoted by dotted lines.

and the modern highly parameterized methods tend to produce density distributions that visibly deviate from the exact ones. Unlike L1, the maximum normalized error of the L2 functionals for electron densities positively correlates with their rung of the Jacob's Ladder (see supplementary materials). Despite their excellent performance for energies and geometries, we must suspect that modern highly parameterized functionals need further guidance from exact constraints, or exact density, or both. For energies and energy differences, the density-driven error (25) could be compensated by the functional error [the error that the approximate functional would make when applied to the exact density, as defined in (25)]. Although their deviation from the exact density is considerable, relative errors in density distributions are small enough to make the trends in resulting integral properties (e.g., atoms-in-molecules charges) similar to trends from MP2 even for a complicated case of a supra-molecular stereoelectronic effect (26).

We also tested our approach to error estimation for electron densities on the well-studied hybrid functional PBE0. The optimal fraction of HF in it was estimated theoretically to be 25% for molecules and their constituent atoms (27). We found that the dependence of atomic normalized errors on HF fraction in the four systems demonstrating the largest errors in our study (Be, Ne, F^{5+} , Ne^{6+}) closely follows the underlying physical model (27) (Fig. 2 and fig. S5): For Be, F^{5+} , and Ne^{6+} , optimum values are close to 25% as proposed for chemically correlated cases, and for weakly correlated Ne the optimum value is close to 50% (although 25% is still reasonable; see Fig. 2). Be, F^{5+} , and Ne^{6+} have relatively small energy gaps between their occupied 2s and unoccupied 2p orbitals, whereas Ne has a huge gap between its occupied 2p and unoccupied 3s orbitals. As the gap increases, the correlation energy becomes

less important compared to the exchange energy, and the optimum fraction of exact exchange increases toward 100%. The overall optimum value is 26.3%, which is very close to the one typically used, and we obtain it without any energy fitting.

We conclude that the latest trend of developing functionals using unconstrained forms leads to unphysical electron densities despite the excellent energy-related performance of these methods. The meta-GGA functionals constructed by the constraint-satisfaction approach produce much better electron densities, and hybrid functionals with physically sound formulations show the best performance. Our findings suggest that the long-neglected electron density will play a crucial role in the future of DFT development. Minimization of deviations from the exact electron density, along with constraint satisfaction and controlled energy fitting, may result in more accurate approximations to the exact functional, providing new computational methods for molecular and solid-state physics. Overall, DFT is in need of new strategies for functional development.

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J.S. contributed the quantum chemical calculations with Gaussian03; J.P.P. and K.A.L. supervised the research; M.G.M. and I.S.B. wrote the paper; and J.S., J.P.P., and K.A.L. edited it. All authors have discussed the results.

SUPPLEMENTARY MATERIALS

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Materials and Methods

Figs. S1 to S5

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Density functional theory is straying from the path toward the exact functional

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Whither the density in DFT calculations?

The continuing development of density functional theory (DFT) has greatly expanded the size and complexity of molecules amenable to computationally tractable simulation. The conventional metric of success for new functionals has been the accuracy of their calculated energies. Medvedev *et al.* examined how well these functionals calculate electron density across a series of neutral and cationic atoms (see the Perspective by Hammes-Schiffer). Although historically the accuracies of energy and density have improved in tandem, certain recent functionals have sacrificed fidelity to the true density.

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