DFT2024 poll

organized by:
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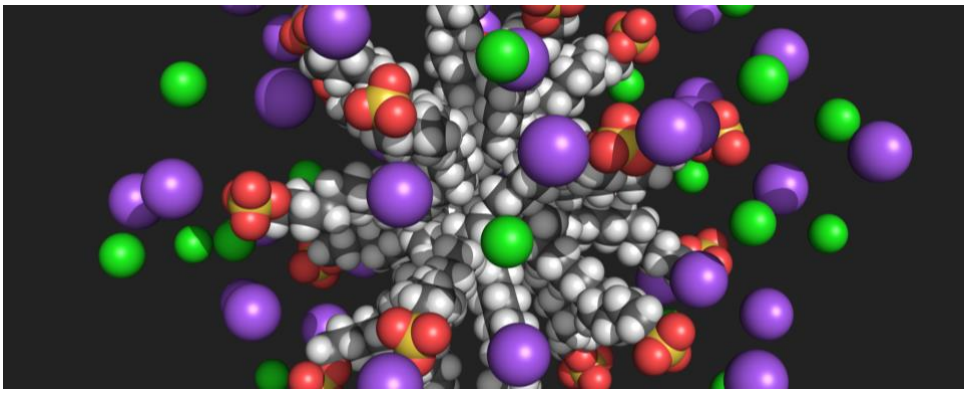


contents

the data:

www.marcelswart.eu/dft-poll

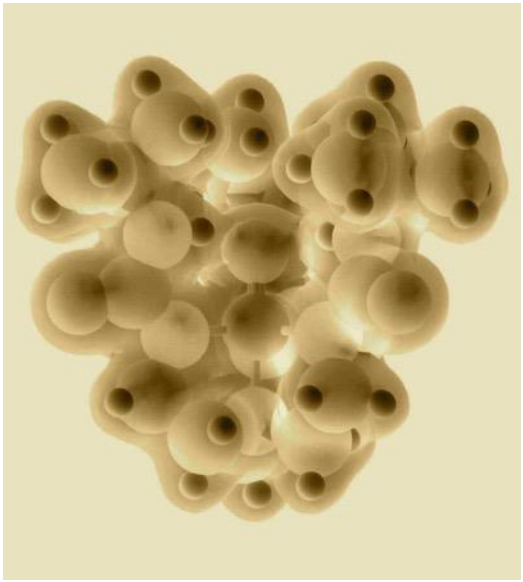
The annual popularity poll for density functionals: **edition 2024**

The 2024 results are in, with a reduction of the number of participation (probably due to unavailability of the Psi-k mailing list over summer): 102 entries. Perdew's functionals remain at the top of the list (PBE **2**, PBE-D **3**, PBE0 **4**), but we have a new favorite functional: **ωB97X-D**.

The other members of the same family are gaining ground as well (now at **5** and **6**). The physics oriented DFAs (HSE, PBEsol, LDA, revPBE) are losing steam, and are relegated to the *Segona Divisió* in 2025.

The following five functionals are promoted to the *Primera Divisió*: B97-3c, B2PLYP, DSD-PBEP86, B97M-V, M06
thereby replacing the following five (that relegate to the *Segona Divisió*):
HSE, PBEsol, SCAN, revPBE, LDA.

There are ten places available for new suggestions to be included. Please send suggestions to marcel.swart@udg.edu before May 15, 2025.



Primera Divisió 2025

B2PLYP, B3LYP, B3LYP-D, B97-3c, B97-D, B97M-V, BP86, CAM-B3LYP, DSD-PBEP86, M06, M06-2X, PBE, PBE-D, PBE0 (PBE1PBE), r2SCAN-3c, r2SCAN-D4, TPSSh, ωB97M-V, ωB97X-D, ωB97X-V

Segona Divisió 2025

B3PW91, BLYP, HSE, LC-PBE, LC-ωPBE, LDA, M06-L, OPBE, optB88-vdW, PBEsol, PW6B95, PW91, PWPB95-D3, revPBE, revTPSS, revTPSS-D, RPA, RPBE, SCAN, SCAN-rVV10

Suggestions

B86bPBE, B97D3, 8 additional slots

Send message to marcel.swart@udg.edu before May 15, 2025 for additional suggestions

news-item

DFT2024 poll

ωB97X-D is most popular

origin of the online popularity poll of density functionals

Following a presentation by Matthias Bickelhaupt (“Hyper-valent versus Nonhypervalent Carbon”, 27. 2. 2009) there was a discussion in Can Paco (the bar at the faculty of Chemistry at the University of Girona). Because the presentation showed the results for quite a number of density functionals, Miquel Duran suggested to take a number of these results, and use appropriate weights for them in order to obtain a “consensus” density functional result. In order to get the weights needed for this procedure, we have held annual online polls where people could indicate their preferences for a number of density functionals. The polls were announced on the CCL and Psi4 lists, on BlueSky, LinkedIn, blogs, etc. in order to get the maximum number of participants. The aims of this poll were: (i) to probe the “preference of the community”, i.e., setting up a ranking of preferred DFT methods; and (ii) provide a compilation of the “de facto quality” that this implies for the “average DFT computation”. Note that this poll does not cover everybody, only those who were motivated to take part in the poll and vote. Yet, we feel that the results do provide some insight in current preferences. And interestingly, these preferences do not always match with the best choice in terms of best agreement with accurate reference data.

density functional theory in a nutshell

In 1964, Hohenberg and Kohn published theorems that laid the basis for density functional theory (DFT). Together with the Kohn-Sham scheme published a year later in 1965, these form the basic framework of DFT. In these papers, it was shown that there exists a one-to-one relation between the energy and density, i.e. it is in principle possible to obtain directly the exact energy from the electron density. But, the mathematical formulation that delivers this energy is unknown, although it can be constructed numerically from an exact (accurate) wavefunction for a concrete system. It was not until the 1980s that the first reasonable approximations were proposed. Apart from the Local Density Approximation (LDA), the Generalized Gradient Approximation (GGA), hybrid functionals containing a portion of *exact* (Hartree-Fock) exchange, meta-GGA functionals, double hybrid functionals, local hybrid functionals, and the hybrid meta-GGA functionals, there are now also the range-separated hybrid functionals.

In 1998, Walter Kohn received the Nobel prize in Chemistry for his work on DFT.

reviews/perspectives

www.marcelswart.eu/dft-poll/reviews.html

Send a message to marcel.swart@udg.edu to have new reviews/perspectives included on the list

The aim of the online popularity poll is to probe the preferences of the computational chemistry and physics communities, and compile the quality of the "average" DFT computation.

Comments 2024 edition:

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references

Kohn-Sham: *Phys. Rev. A 1965, 140, 1133*

Hohenberg-Kohn: *Phys. Rev. B 1964, 136, 864*

APBE: *Phys. Rev. Lett. 2011, 106, 186406*

B2PLYP: *J. Chem. Phys. 2006, 124, 034108*

B3LYP: *J. Phys. Chem. 1994, 98, 11623*

B3LYP-D: *J. Phys. Chem. 1994, 98, 11623; J. Comput. Chem. 2006, 27, 1787*

B3LYP*: *Theor. Chem. Acc. 2001, 107, 48*

B3PW91: *J. Chem. Phys. 1993, 98, 5648*

ωB97X-D: *Phys. Chem. Chem. Phys. 2008, 10, 6615*

B97-D: *J. Comput. Chem. 2006, 27, 1787*

BHandH: *J. Chem. Phys. 1993, 98, 1372*

BLYP: *Phys. Rev. A 1988, 38, 3098; Phys. Rev. B 1988, 37, 785*

BP86: *Phys. Rev. A 1988, 38, 3098; Phys. Rev. B 1986, 33, 8822*

CAM-B3LYP: *Chem. Phys. Lett. 2004, 393, 51*

DSD-BLYP: *J. Phys. Chem. C 2010, 114, 20801*

DSD-PBEP86: *Phys. Chem. Chem. Phys. 2011, 13, 20104*

HSE: *J. Chem. Phys. 2003, 118, 8207*

KT1: *J. Chem. Phys. 2003, 119, 3015*

LB94: *Phys. Rev. A 1994, 49, 2421*

LC-ωPBE: *J. Chem. Phys. 2006, 125, 234109*

LC-PBE: *J. Chem. Phys. 2007, 126, 154105*

LDA: *Proc. Roy. Soc. (London) A 1929, 123, 714; Phys. Rev. 1951, 81, 385; Can. J. Phys. 1980, 58, 1200; Phys. Rev. B 1992, 45, 13244*

M05: *J. Chem. Phys. 2005, 123, 161103*

M05-2X: *J. Chem. Theory Comput. 2006, 2, 364*

M06, M06-2X: *Theor. Chem. Acc. 2008, 120, 215*

M06-L: *J. Chem. Phys. 2006, 125, 194101*

mPW1K: *J. Phys. Chem. A 2000, 104, 4811*

MVS: *PNAS 2015, 112, 685*

OLYP: *Mol. Phys. 2001, 99, 403; Phys. Rev. B 1988, 37, 785*

optB88-vdW: *J. Phys.-Condens. Mat. 2010, 22, 022201*

PBE: *Phys. Rev. Lett. 1996, 77, 3865*

PBE0: *J. Chem. Phys. 1996, 105, 9982; J. Chem. Phys. 1999, 110, 5029; J. Chem. Phys. 1999, 110, 6158*

PW6B95: *J. Phys. Chem. A 2005, 109, 5656*

PW91: *Phys. Rev. B 1992, 46, 6671*

PWPB95-D$_3$: *J. Chem. Theory Comput. 2011, 7, 291*

revPBE: *Phys. Rev. Lett. 1998, 80, 890*

revTPSS, revTPSS-D: *Phys. Rev. Lett. 2009, 103, 026403; s_6=0.7282 (revTPSS-D)*

RPA: *J. Chem. Phys. 2008, 129, 114105*

RPBE: *Phys. Rev. B 1999, 59, 7413*

S12g, S12h: *Chem. Phys. Lett. 2013, 580, 166*

SAOP: *J. Chem. Phys. 2000, 112, 1344*

SCAN: *Phys. Rev. Lett. 2015, 115, 036402*

SSB-D: *J. Chem. Phys. 2009, 131, 094103*

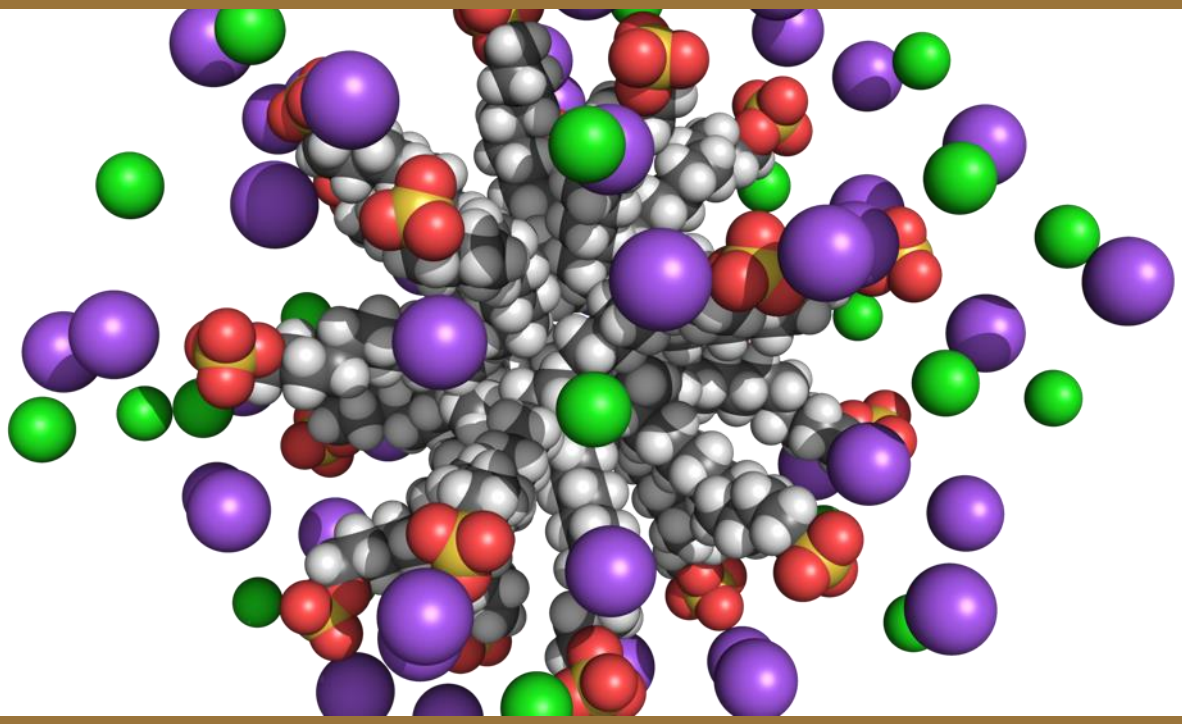
τ-HCTH: *J. Chem. Phys. 2002, 116, 9559*

TPSSh: *Phys. Rev. Lett. 2003, 91, 146401; J. Chem. Phys. 2003, 119, 12129*

VSXC: *J. Chem. Phys. 1998, 109, 400*

Comments

- [Functional] + [XDM, TS, MBD]
- For transition metal, I like B3LYP and BP86 and for main group chemistry, M062X
- None of the above = I haven't used it before.
- B86bPBE
- "As evidenced by the references, e.g., ""B3LYP-D"" is not really a separate functional, but simply B3LYP, together with one specific version of Grimme's dispersion correction. A dispersion correction should always be used, but whether this specific one, or a more recent version like D4, or a non-local correlation functional like VV10, is a separate question. Similarly, Chai and Head-Gordon's wB97X-D refit is not particularly impressive, but the wB97X-V functional with a drop-in replacement of VV10 by D3(BJ) or D4 is rather good. Lumping nuanced factors like that into a single (Gaussian-flavored) keyword is likely to skew the results of the poll."



- Missing the mention of MBD
- I am neutral on all functionals that did not test myself. But I cannot say I really enjoy a particular functional since there's no exact one at all.
- B97D3
- Include TPSSh
    - **It has been included since the beginning. See: https://www.marcelswart.eu/dft-poll/TPSSh.html**
- Few new ones in there for me to go explore. Thanks.