DFT2020 poll

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contents

the data:

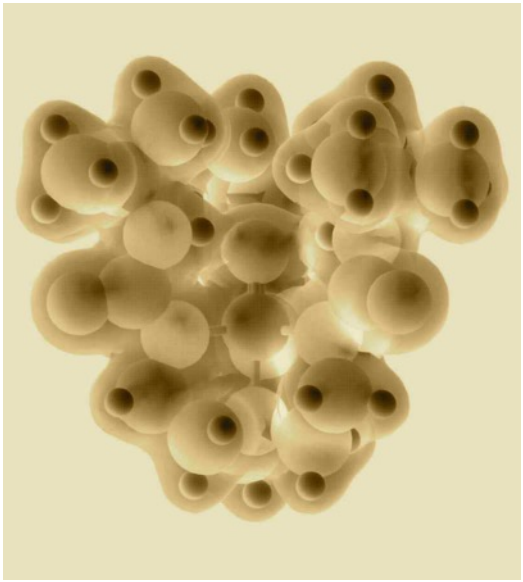
www.marcelswart.eu/dft-poll

The annual popularity poll for density functionals: **edition 2020**

The 2020 results are in, with a record number of participation: **253 entries**! Perdew's functionals remain at the top of the list (PBE **1**, PBE0 **2**, PBE-D **4**), with ωB97X-D consolidating in the *Primera Divisió* at number **3**. The Minnesota functionals and LDA are losing steam again (M06-2X down to **13**, LDA to **12**), while BP86 continues its struggles (now at place **16**, thereby relegating again to *Segona Divisió*). (full results available online)

The following five functionals are promoted to the *Primera Divisió*:
SCAN, TPSSh, revTPSS, revTPSS-D, M06
thereby replacing the following five (that relegate to the *Segona Divisió*):
BP86, RPA, LC-ωPBE, B2PLYP, BLYP.

Several new contestants have already been put forward through the comments: MS, MN15L, SCAN-rVV10, r2SCAN-D4, PBE-uMBD, TASKxc, RevDOD-PBEP86-D



PBE continues its success

Primera Divisió 2021

B3LYP, B3LYP-D, B97-D, CAM-B3LYP, HSE, LDA, M06, M06-2X, PBE, PBE-D, PBE0 (PBE1PBE), PBEsol, PW91, revPBE, revTPSS, revTPSS-D, SCAN, TPSSh, ωB97X-D, ωB97X-V

Segona Divisió 2021

B2PLYP, B3PW91, B97-3c, B97M-V, BEEF-vdW, BLYP, BP86, DSD-BLYP, DSD-PBEP86, LC-PBE, LC-ωPBE, M06-L, OLYP, optB88-vdW, PW6B95, PWPB95-D3, RPA, RPBE, S12g, wB97M-V

Suggestions

MS, MN15L, SCAN-rVV10, r2SCAN-D4, PBE-uMBD, TASKxc, RevDOD-BLYP-D, 3 additional slots

Send message to marcel.swart@udg.edu for additional suggestions

news-item

DFT2020 poll

origin of the online popularity poll of density functionals

Following a presentation by Matthias Bickelhaupt ("Hypervalent 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 list, on Twitter, Facebook, 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.

Girona, Amsterdam

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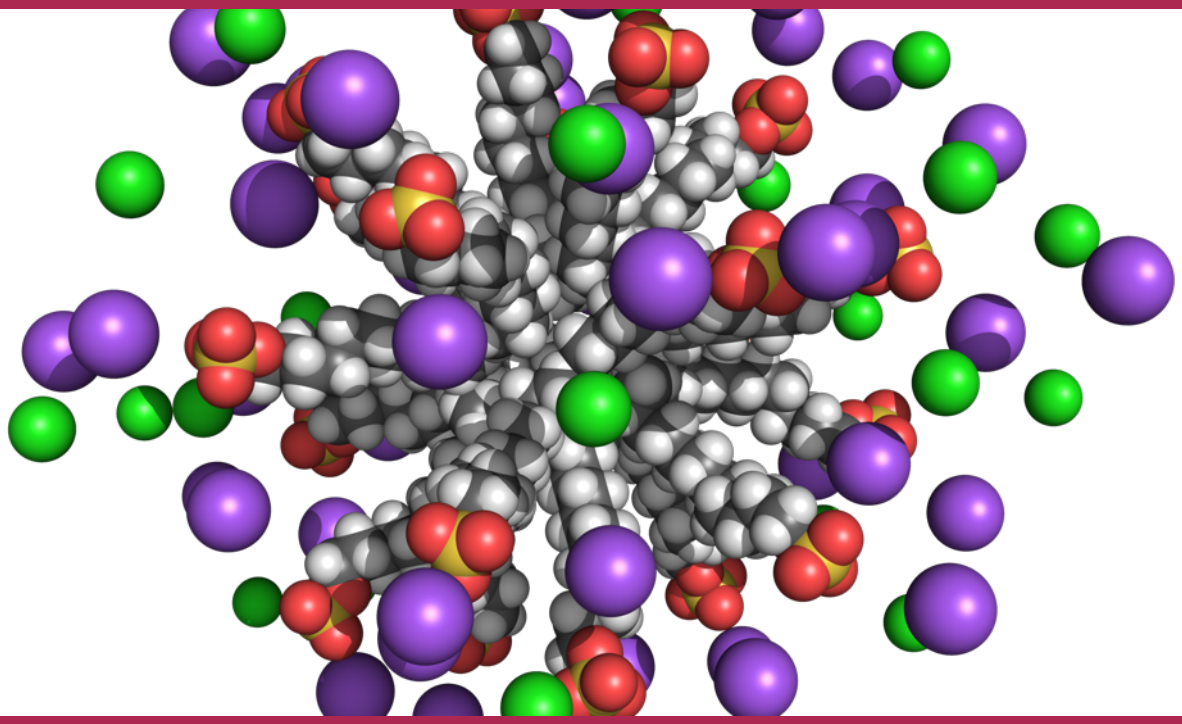
General comments

- It's a little hard to rank a functional with and without -D. I feel like with the ubiquity of dispersion corrections these days, it might be worth voting under the assumption that a D correction can be applied if desired.
- In my experience PBE0 give better results with similar computational cost as HSE06 and others are sophisticated but too much in demand for computer power (of course LDA, PBE are still very cheap)
- SCAN is very hard to converge with slab + vacuum!!!!!!!
- I consistently find that CAM-B3LYP is good for TD-DFT of transition metal complexes, M06-2X for main group mechanistic studies, B3LYP good for organic molecules (good = most replicates experimental data).
- There no reason for hate



Proposed new functionals to be included

- I would like to suggest the MS (made simple) MGGA and vdW-DF1/2/3 functionals
- wB97M(2)
- Like MN15L
- RevDOD-BLYP-D RevDOD-PBEP86-D RecDOD-PBEPBE-D
- revDOD-BLYP-D revDODPBEPBE-D revDODPBEP86-D
- SCAN-rVV10 should be in the list
- PBE0-DH best of the double hybrids
- New favourite = rSCAN - not in your list?
- PBEh-3c
- What about SCAN or optb86b and vdW-DF functionals?