DFT2019 poll

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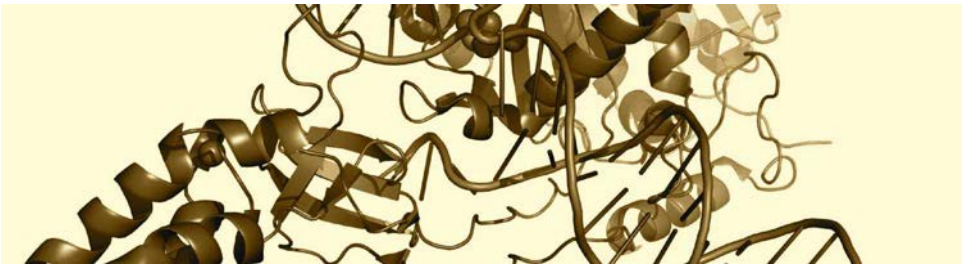


contents

the data:

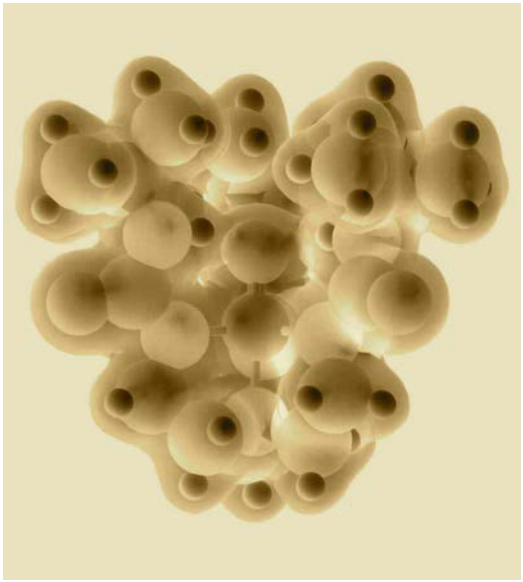
www.marcelswart.eu/dft-poll

The annual popularity poll for density functionals: **edition 2019**

The 2019 results are in. And what an amazing number of them! **232 entries**, the largest number of participants in our 10 years of polling the community. Perdew's functionals remain at the top of the list (PBE **1**, PBE0 **2**, PBE-D **5**), with LDA coming back strongly in the *Primera Divisió* at number 7. The Minnesota functionals are slowly going up (M06-2X **9**) and going down (M06-L/M06 **18**/**19**, relegating to *Segona Divisió*). (full results available online)

This year is the first edition where we return to the initial setup, without a third question. Without any doubt this has had its influence on the number of participants.

The following five functionals are promoted to the *Primera Divisió*: BP86, BLYP, PBEsol, RPA, LC-ωPBE
thereby replacing the following five (that relegate to the *Segona Divisió*):
SCAN, TPSSh, M06-L, M06, DSD-PBEP86.



PBE continues its success

Primera Divisió 2020

B2PLYP, B3LYP, B3LYP-D, B97-D, BLYP, BP86, CAM-B3LYP, HSE, LC-ωPBE, LDA, M06-2X, PBE, PBE-D, PBE0 (PBE1PBE), PBEsol, PW91, revPBE, RPA, ωB97X-D, ωB97X-V

Segona Divisió 2020

B3PW91, B97-3c, B97M-V, BEEF-vdW, BHandH, DSD-BLYP, DSD-PBEP86, LC-PBE, M06, M06-L, OLYP, optB88-vdW, PW6B95, PWPB95-D3, revTPSS, revTPSS-D, RPBE, SCAN, TPSSh, wB97M-V

Suggestions

S12g, MN15, 8 additional slots

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

news-item

DFT2019 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.

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references

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

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

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

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***MVS**: PNAS 2015, 112, 685*

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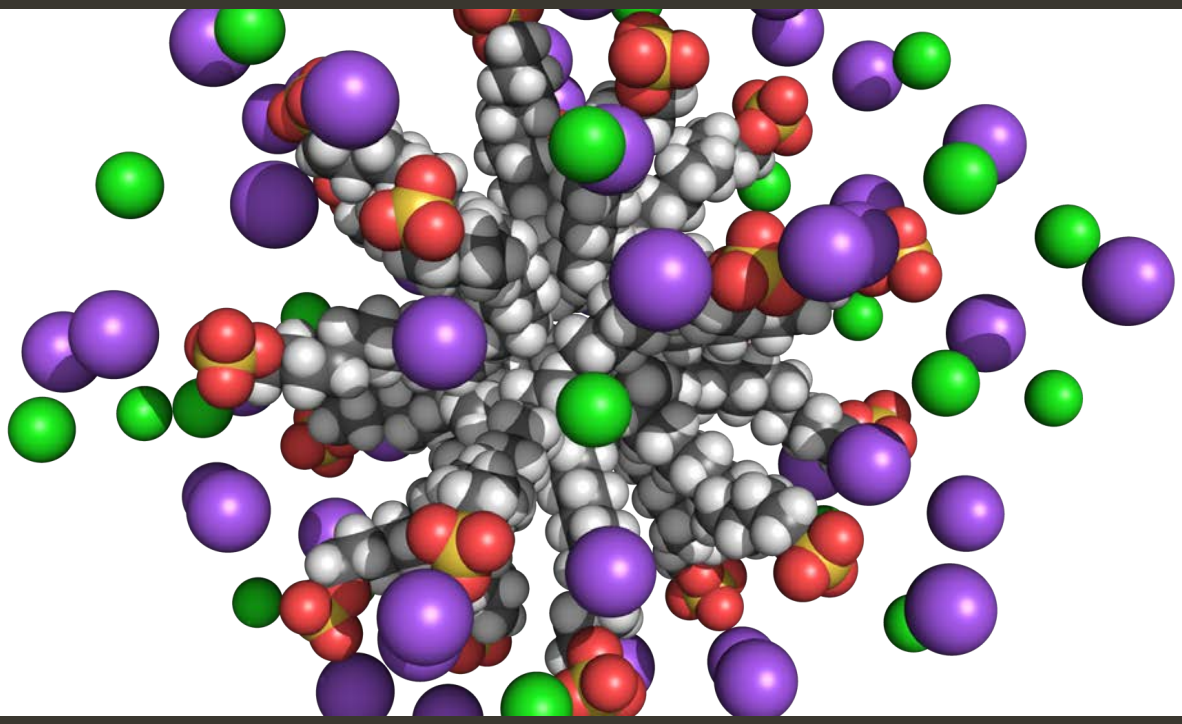
Ten years polling the community

In these 10 years of holding the DFT poll, we have seen:

- a total of **54 functionals** and **1348 participants** that have entered the equations
- static functionals (e.g. PBE, PBE0) vs. mobile functionals (e.g. LDA, BLYP, M06-L)
- a total of **30219 points** been given (20828 *Primera*, 9391 *Segona*)
    - an average of 22.4 points per candidate per year: 15.4 *Primera*, 7.0 *Segona*
- an average of **26.6 votes per candidate**
    - 5.9 likes, 8.9 neutral, 4.1 hate
        - *Primera*: 14.3 votes, 4.3 likes, 4.9 neutral, 2.3 hate
        - *Segona*: 12.4 votes, 1.6 likes, 4.0 neutral, 1.8 hate



Outstanding functionals

Top10	Most **Points**	Most **Likes**	Most **Neutrals**	Most **Hates**	Most **Votes**
1	PBE	PBE	B3PW91	M06-2X	B3LYP
2	PBE0	PBE0	PW91	B3LYP	PBE
3	B3LYP	B3LYP	BLYP	M06-L	PBE0
4	BP86	M06-2X	B97-D	LDA	LDA
5	wB97X-D	LDA	CAM-B3LYP	M06	M06-2X
6	B3LYP-D	BP86	B2PLYP	BLYP	CAM-B3LYP
7	LDA	wB97X-D	TPSSh	M05-2X	M06-L
8	CAM-B3LYP	B3LYP-D	OLYP	BHandH	BP86
9	M06-2X	CAM-B3LYP	revTPSS	B3LYP-D	B97-D
10	B97-D	B97-D	BHandH	B3LYP*	BLYP