DFT2018 poll

organized by:
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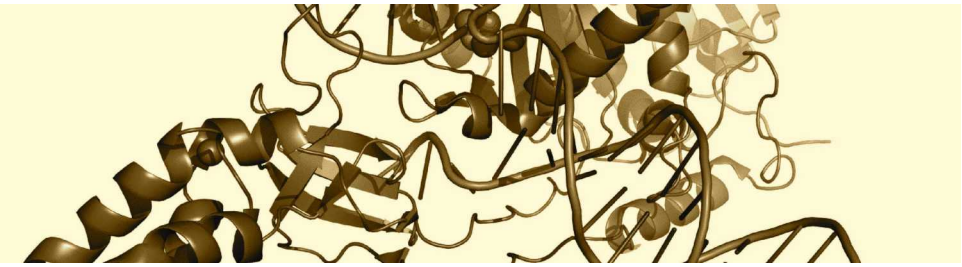


contents

the data:

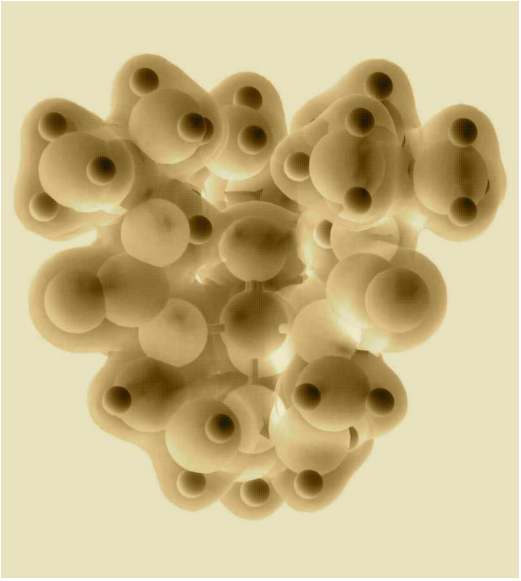
www.marcelswart.eu/dft-poll

The annual popularity poll for density functionals: **edition 2018**

The 2018 results are in. And they are **astonishing!** We have a new number one: PBE, with the previous number 1 still going strong at 2 (PBE0/PBE1PBE). The big surprise is however PBE-D that rushes in, and in its first year in the Primera Divisió claims the third spot!! (full results available online)

Surprisingly enough, the winner (PBE) does not feature at all in the top 10 for any of the eleven properties of the third question. Hence, there is no consistency between questions 1-2 and question 3, and the organization decided to go back to the original design of the poll with only two questions.

The following five functionals are promoted to the **Primera Divisió**: LDA, M06-L, M06, SCAN, DSD-PBEP86
thereby replacing the following five (that relegate to the **Segona Divisió**): PWPB95-D3, wB97M-V, LC-wPBE, BP86, B97M-V.



PBE reclaims top spot

Primera Divisió 2019

B2PLYP, B3LYP, B3LYP-D, B97-D, CAM-B3LYP, DSD-PBEP86, HSE, LDA, M06, M06-2X, M06-L, PBE, PBE-D, PBE0 (PBE1PBE), PW91, revPBE, SCAN, TPSSh, wB97X-D, wB97X-V

Segona Divisió 2019

B3PW91, B97M-V, BEEF-vdW, BHandH, BLYP, BP86, DSD-BLYP, LC-PBE, LC-wPBE, OLYP, optB88-vdW, PBEsol, PW6B95, PWPB95-D3, revTPSS, revTPSS-D, RPA, RPBE, S12g, SAOP, SSB-D, wB97M-V

Suggestions

PBEsol, BEEF-vdW, 8 additional slots

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

news-item

DFT2018 poll

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 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.

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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