DFT2023 poll

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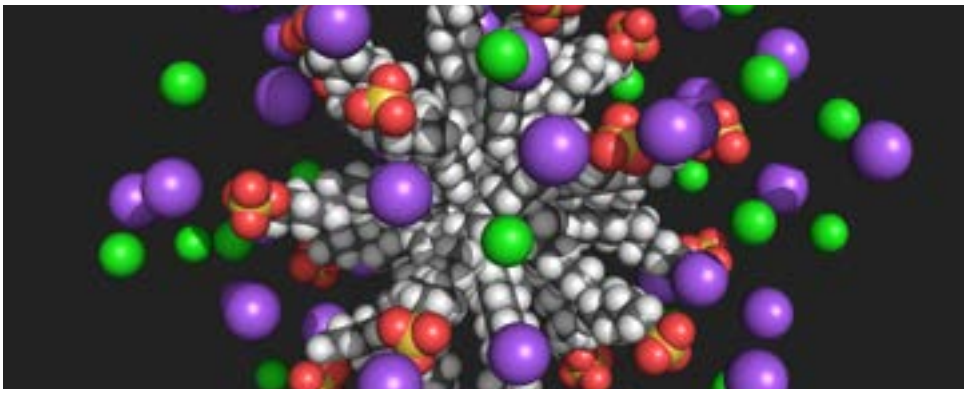


contents

the data:

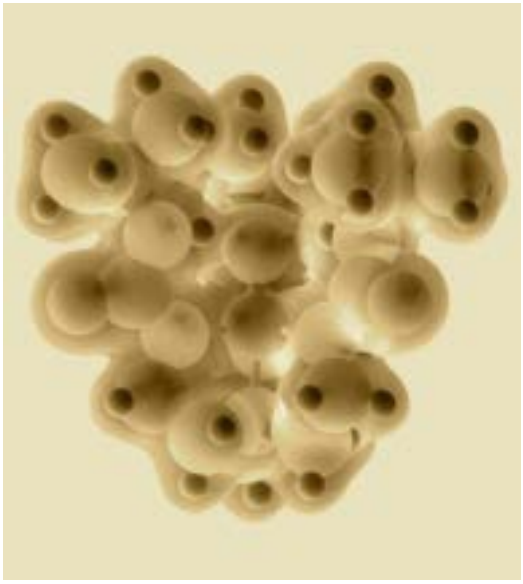
www.marcelswart.eu/dft-poll

The annual popularity poll for density functionals: **edition 2023**

The 2023 results are in, with a reduction of the number of participation: 166 entries. Perdew's functionals remain at the top of the list (PBE **1**, PBE-D **3**, PBE0 **4**, PBEsol **6**), with ωB97X-D gaining track again in the *Primera Divisió* (jumping from number **4** to number **2**). HSE has lost its steam a bit, and is now found at number **7**, while PBEsol remains high in the ranking (now at **6**). LDA lost its top10 spot (now at place **12**), while the Minnesota functionals are losing steam (M06 and M06-L remain in the *Segona Divisió* next year, but MN15 and MN12SX are out), yet M06-2X returns to the *Primera Divisió* next year. (full results available online)

The following five functionals are promoted to the *Primera Divisió*:
M06-2X, BP86, TPSSh, revPBE, r2SCAN-3c
thereby replacing the following five (that relegate to the *Segona Divisió*):
SCAN-rVV10, PW91, B97M-V, RPA, B97-3c.

There are ten places available for new suggestions to be included.



Primera Divisió 2024

B3LYP, B3LYP-D, B97-D, BP86, CAM-B3LYP, HSE, LDA, M06-2X, PBE, PBE-D, PBE0 (PBE1PBE), PBEsol, r2SCAN-3c, r2SCAN-D4, revPBE, SCAN, TPSSh, ωB97M-V, ωB97X-D, ωB97X-V

Segona Divisió 2024

B2PLYP, B3PW91, B97-3c, B97M-V, BLYP, DSD-PBEP86, LC-PBE, LC-ωPBE, M06, M06-L, OPBE, optB88-vdW, PW6B95, PW91, PWPB95-D3, revTPSS, revTPSS-D, RPA, RPBE, SCAN-rVV10

Suggestions

10 additional slots

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

news-item

DFT2023 poll

PBE continues its success

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 2023 edition:
- **none**

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references

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

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

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

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

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

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

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

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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*

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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*

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

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

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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*

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