Supplementary Information: Thirty years of density functional theory in computational chemistry: An overview and extensive assessment of 200 density functionals

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I. THE 200 FUNCTIONALS

If a dispersion-corrected functional is not cited, it means that its parent functional already has the necessary citations and the only additional citation is covered under the "Citations for Dispersion Components" heading. For example, B3LYP is properly cited below, while B3LYP-D2 is not, since the D2 parameterization for B3LYP is covered in the citation given for D2. If a dispersion-corrected functional is cited, this means that the parameters for the dispersion correction were determined in the cited paper and not in the citation given under "Citations for Dispersion Components".

Citations for Dispersion Components
D2[1]
D3(0)[2]
D3(BJ)[3]
D3(CSO)[4]
D3M(BJ)[5]
VV10[6]
rVV10[7]
[†] dftd3.f from DFT-D3 V3.2 Rev 0

Local – LSDA (2)
SVWN5[8]
SPW92[9]

Local – GGA (61)
B97-D[1]
B97-D3(0)
B97-D3(BJ)
B97-D3M(BJ)
BLYP[10,11]
BLYP-D2
BLYP-D3(0)
BLYP-D3(BJ)
BLYP-D3(CSO)
BLYP-D3M(BJ)
BLYP-NL[12]
BOP[10,13]
BOP-D3(0)[†]
BOP-D3(BJ)[†]
BP86[10,14]

BP86-D2
BP86-D3(0)
BP86-D3(BJ)
BP86-D3(CSO)
BP86-D3M(BJ)
BPBE[10,15]
BPBE-D3(0)[†]
BPBE-D3(BJ)[†]
GAM[16]
HCTH/93[17]
HCTH/120[18]
HCTH/120-D3(0)[†]
HCTH/120-D3(BJ)[†]
HCTH/147[18]
HCTH/407[19]
mPW91[20,21]
N12[22]
N12-D3(0)[23]
OLYP[11,24]
OLYP-D3(0)[†]
OLYP-D3(BJ)[†]
PBE[15]
PBE-D2
PBE-D3(0)
PBE-D3(BJ)
PBE-D3(CSO)
PBE-D3M(BJ)
PBEOP[13,15]
PBEsol[25]
PBEsol-D3(0)[†]
PBEsol-D3(BJ)[†]
PW91[21]
revPBE[15,26]
revPBE-D2[†]
revPBE-D3(0)
revPBE-D3(BJ)
revPBE-NL[12]
RPBE[15,27]
RPBE-D3(0)[†]
RPBE-D3(BJ)[†]
rPW86PBE[15,28]
rPW86PBE-D3(0)[†]
rPW86PBE-D3(BJ)
rVV10[7]
SOGGA[15,29]
VV10[6]

Local − meta-GGA (35)
B97M-V[30]
B97M-rV[31]
BLOC[32]
BLOC-D3(0)[32]
M06-L[33]
M06-L-D2[34]
M06-L-D3(0)[†]
M11-L[35]
M11-L-D3(0)[23]
mBEEF[25,36]
MN12-L[37]
MN12-L-D3(BJ)[23]
MN15-L[38]
MS0[39]
MS0-D3(0)[40]
MS1[40]
MS1-D3(0)[40]
MS2[40]
MS2-D3(0)[40]
MVS[41]
oTPSS-D3(0)[42]
oTPSS-D3(BJ)[†]
PKZB[43]
revTPSS[44]
SCAN[45]
SCAN-D3(0)[46]
SCAN-D3(BJ)[46]
SCAN+rVV10[47]
TM[48]
TPSS[49]
TPSS-D2
TPSS-D3(0)
TPSS-D3(BJ)
TPSS-D3(CSO)
τ-HCTH[50]

Global Hybrid − None (4)
HF
HF-D3(0)[†]
HF-D3(BJ)
HF-NL[12]

Global Hybrid − LSDA (1)
HFPW92[9]

Global Hybrid − GGA (33)
B3LYP[8,10,11,51]
B3LYP-D2
B3LYP-D3(0)
B3LYP-D3(BJ)
B3LYP-D3(CSO)
B3LYP-D3M(BJ)
B3LYP-NL[12]
B3P86[8,10,14,51]
B3PW91[9,10,21,51]
B3PW91-D2[34]
B3PW91-D3(0)[†]
B3PW91-D3(BJ)[†]
B97[52]

B97-1[17]
B97-1-D2[34]
B97-2[53]
B97-2-D2[34]
B97-3[54]
B97-3-D2[34]
B97-D2[55]
B97-K[56]
HFLYP[11]
PBE0[57]
PBE0-D2[34]
PBE0-D3(0)
PBE0-D3(BJ)
PBE0-D3(CSO)
PBE0-D3M(BJ)
revPBE0[15,26,57]
revPBE0-D3(0)[†]
revPBE0-D3(BJ)[†]
SOGGA11-X[58]
SOGGA11-X-D3(BJ)[23]

Global Hybrid − meta-GGA (37)
BMK[56]
BMK-D2[34]
BMK-D3(0)[†]
BMK-D3(BJ)[†]
M05[59]
M05-D3(0)[†]
M05-2X[60]
M05-2X-D3(0)[†]
M06[61]
M06-D2[34]
M06-D3(0)[†]
M06-2X[61]
M06-2X-D2[34]
M06-2X-D3(0)[†]
M06-HF[62]
M06-HF-D3(0)[†]
M08-HX[63]
M08-SO[63]
MN15[64]
MS2h[40]
MS2h-D3(0)[40]
MVSh[41]
PW6B95[65]
PW6B95-D2[34]
PW6B95-D3(0)
PW6B95-D3(BJ)
PW6B95-D3(CSO)
PWB6K[65]
PWB6K-D3(0)[†]
PWB6K-D3(BJ)[†]
revTPSSh[66]
SCAN0[67]
TPSSh[68]
TPSSh-D2[34]
TPSSh-D3(0)[†]
TPSSh-D3(BJ)[†]
τ-HCTHh[50]

Range-Separated Hybrid – GGA (20)
CAM-B3LYP[69]
CAM-B3LYP-D3(0)[†]
CAM-B3LYP-D3(BJ)[†]
HSE-HJS[15,70,71]
HSE-HJS-D3(0)[†]
HSE-HJS-D3(BJ)[†]
LC-VV10[6]
LC-ωPBE08[72]
LC-ωPBE08-D3(0)[†]
LC-ωPBE08-D3(BJ)[†]
LC-ωPBE08-D3M(BJ)
LRC-ωPBE[73]
LRC-ωPBEh[73]
N12-SX[74]
N12-SX-D3(BJ)[23]
ωB97[75]
ωB97X[75]
ωB97X-D[76]
ωB97X-D3[77]
ωB97X-V[78]

Range-Separated Hybrid – meta-GGA (7)
M11[79]
M11-D3(BJ)[23]
MN12-SX[74]
MN12-SX-D3(BJ)[23]
ωB97M-V[80]
ωM05-D[81]
ωM06-D3[77]

II. MGCDB84 DATABASE

The origins of the reference values used for the 84 datasets are further explained here:

- The **A24** reference values are taken from Table 1 of Reference 82 by adding the CCSD(T)/CBS and core correlation columns.

- The **DS14** reference values are taken from Table 1 of Reference 83 from the CBS $(\Delta aTZ)^b$ column.

- The **HB15** reference values are taken from Table S1 of the SI of Reference 84.

- The **HSG** reference values are taken from Table 6 of Reference 85 from the "HSG-A" column.

- The **NBC10** reference values are taken from NBC10.txt of the SI of Reference 85.

- The **S22** reference values are taken from Table 1 of Reference 85.

- The **X40** reference values are taken from Table 1 of Reference 86. The dimers that contain iodine have been removed.

- The **A21x12** reference values were acquired from the authors of Reference 87.

- The **BzDC215** reference values are taken from the SI of Reference 88.

- The **HW30** reference values are taken from Table 1 of Reference 89 from the "$E_{int}^{CCSD(T)\ c}$" column.

- The **NC15** reference values are taken from Table S1 of the SI of Reference 90. The LiH dimer and the five duplicate dimers from A24 have been removed.

- The **S66** reference values are taken from BEGDB.com from the "CCSD(T)/CBS(haTZ) CP" column.

- The **S66x8** reference values are taken from BEGDB.com from the "CCSD(T)/CBS CP" column.

- The **3B-69-DIM** reference values are taken from Table S1 of the SI of Reference 91.

- The **AlkBind12** reference values are taken from Tables 1-3 of Reference 92. The non-counterpoise-corrected CCSD(T)/CBS values are used.

- The **CO2Nitrogen16** reference values are taken from the BENCHMARK folder in the SI of Reference 93. Only the equilibrium geometries (1.0) are used.

- The **HB49** reference values are taken from Table 8 of Reference 94.

- The **Ionic43** reference values are taken from Tables 1 and 2 of Reference 95. Ionic43 is a combination of the AHB21, CHB6, and IL16 datasets.

- The **H2O6Bind8** reference values are taken from Table S4 of the SI of Reference 96 from the "CCSD(T)/CBS" column.

- The **HW6Cl** reference values are taken from Table S7 of the SI of Reference 96 from the "CCSD(T)/CBS" column.

- The **HW6F** reference values are taken from Table S6 of the SI of Reference 96 from the "CCSD(T)/CBS" column.

- The **FmH2O10** reference values are taken from Table S8 of the SI of Reference 96 from the "CCSD(T)/CBS" column.

- The **Shields38** reference values are taken from BEGDB.com from the "CCSD(T)/CBS noCP" column.

- The **SW49Bind345** reference values are taken from Table 1 of the SI of Reference 97.

- The **SW49Bind6** reference values are taken from Table 1 of the SI of Reference 97.

- The **WATER27** reference values are taken from GMTKN30. The 4 water 20-mers have been removed and placed in H2O20Bind4.

- The **3B-69-TRIM** reference values are constructed by combining the three-body energies from the CCSD(T)/CBS column of Table 1 of Reference 91 with the two-body energies from 3B-69-DIM.

- The **CE20** reference values are taken from Table S2 of the SI of Reference 98 from the "ΔE_e^d" column.

- The **H2O20Bind10** reference values are taken from Table S5 of the SI of Reference 96 from the "CCSD(T)/CBS" column.

- The **H2O20Bind4** reference values are taken from the abstract of Reference 99.

- The **TA13** reference values are taken from Table 1 of Reference 100 from the "E_{nonrel}^a" column.

- The **XB18** reference values are taken from the "Energies XB18" tab of the SI (ct301064t_si_001.xlsx) of Reference 101. The values under "REFERENCE CCSD(T)/CBS" are used. The systems with iodine are removed.

- The **Bauza30** reference values are taken from Table 1 of Reference 102 from the "Ave-CBS" column.

- The **CT20** reference values are taken from Table S5 of the SI of Reference 103 from the "CCSD(T)" column.

- The **XB51** reference values are taken from the "WF on XB51" tab of the SI (ct301064t_si_001.xlsx) of Reference 101. The values under "CCSD(T)/AVTZ MP2-CBS(Q5)" are used. The systems with iodine, palladium, and lithium are removed.

- The **AlkIsomer11** reference values are taken from Table S8 of the SI of Reference 34.

- The **Butanediol65** reference values are taken from the "Energies" tab of the SI (jp410723v_si_001.xlsx) of Reference 104. The values under "CCSD(T)-F12b cc-pVTZ-F12" are used.

- The **ACONF** reference values are taken from GMTKN30.

- The **CYCONF** reference values are taken from GMTKN30.

- The **Pentane14** reference values are taken from Table 1 of Reference 105 from the "CCSD(T)" column.

- The **SW49Rel345** reference values are taken from Table 1 of the SI of Reference 97.

- The **SW49Rel6** reference values are taken from Table 1 of the SI of Reference 97.

- The **H2O16Rel5** reference values are taken from Table 1 of Reference 106 from the "ΔE_e [CCSD(T)]" column.

- The **H2O20Rel10** reference values are relative binding energies of the H2O20Bind10 dataset.

- The **H2O20Rel4** reference values are relative binding energies of the H2O20Bind4 dataset.

- The **Melatonin52** reference values are taken from Table 1 of Reference 107 from the "best" column.

- The **YMPJ519** reference values are taken from the SI (ESI_2_DFT-new with CV.xlsx within ct5b01066_si_002.zip) of Reference 108 from the Reference tab with CV on.

- The **EIE22** reference values are taken from Table 1 of Reference 109 from the "ΔE_e^e" column.

- The **Styrene45** reference values are taken from Table 1 of Reference 110 from the "ΔE_e^d" column.

- The **DIE60** reference values are taken from Table 1 of Reference 111 from the "ΔE_e^e" column.

- The **ISOMERIZATION20** reference values are taken from the SI (mmc1.xls) of Reference 112 from the Table SI-VIII tab and the "TAEe (a)" column.

- The **C20C24** reference values are taken from Table 5 of Reference 113 from the "MP2-F12/VTZ-F12+HLC/VTZ" column.

- The **AlkAtom19** reference values are taken from Table S7 of the SI of Reference 34.

- The **BDE99nonMR** reference values are taken from the SI (mmc1.xls) of Reference 112 from the Table SI-VI tab and the "TAEe (a)" column.

- The **G21EA** reference values are taken from GMTKN30.

- The **G21IP** reference values are taken from GMTKN30.

- The **TAE140nonMR** reference values are taken from the SI (mmc1.xls) of Reference 112 from the Table SI-V tab and the "TAEe (a)" column.

- The **AlkIsod14** reference values are taken from Table S9 of the SI of Reference 34.

- The **BH76RC** reference values are taken from GMTKN30.

- The **EA13** reference values are taken from http://comp.chem.umn.edu/db/dbs/ea13.html from the "REF1" column.

- The **HAT707nonMR** reference values are taken from the SI (mmc1.xls) of Reference 112 from the Table SI-VII tab and the "TAEe (a)" column.

- The **IP13** reference values are taken from http://comp.chem.umn.edu/db/dbs/ip21.html from the "REF1" column. Only the first 13 entries are taken.

- The **NBPRC** reference values are taken from GMTKN30.

- The **SN13** reference values are taken from the SI (mmc1.xls) of Reference 112 from the Table SI-IX tab and the "TAEe (a)" column.

- The **BSR36** reference values are taken from GMTKN30.

- The **HNBrBDE18** reference values are taken from Table 1 of Reference 114 from the "$BDE_e^{[a]}$" column.

- The **WCPT6** reference values are taken from Table 1 of Reference 115.

- The **BDE99MR** reference values are taken from the SI (mmc1.xls) of Reference 112 from the Table SI-VI tab and the "TAEe (a)" column.

- The **HAT707MR** reference values are taken from the SI (mmc1.xls) of Reference 112 from the Table SI-VII tab and the "TAEe (a)" column.

- The **TAE140MR** reference values are taken from the SI (mmc1.xls) of Reference 112 from the Table SI-V tab and the "TAEe (a)" column.

- The **PlatonicHD6** reference values are taken from Table 1 of Reference from the "$TAE_e^{[f]}$" row.

- The **PlatonicID6** reference values are taken from Table 1 of Reference from the "$TAE_e^{[f]}$" row.

- The **PlatonicIG6** reference values are taken from Table 1 of Reference from the "$TAE_e^{[f]}$" row.

- The **PlatonicTAE6** reference values are taken from Table 1 of Reference from the "$TAE_e^{[f]}$" row.

- The **BHPERI26** reference values are taken from Table S3 of the SI of Reference 116 from the ΔE_e^c column.

- The **CRBH20** reference values are taken from Table 2 of Reference 117 from the "ΔE_e^c" column.

- The **DBH24** reference values are taken from Table 1 of Reference 118 from the "TAE_e^a" column.

- The **CR20** reference values are taken from Table 2 of Reference 119 from the "ΔE_e^c" column.

- The **HTBH38** reference values are taken from GMTKN30.

- The **NHTBH38** reference values are taken from GMTKN30.

- The **PX13** reference values are taken from Table S2 of the SI of Reference 98 from the "ΔE_e^d" column.

- The **WCPT27** reference values are taken from Table 1 of Reference 115.

- The **AE18** reference values are taken from Table 11 of Reference 120 from the last column of each row.

- The **RG10** reference values are generated using the Tang-Toennies model in Reference 121. HeHe ranges from 2 to 8 Å. HeNe ranges from 2 to 8 Å. HeAr ranges from 2.2 to 8 Å. HeKr ranges from 2.3 to 8 Å. NeNe ranges from 2 to 8 Å. NeAr ranges from 2.4 to 8 Å. NeKr ranges from 2.5 to 8 Å. ArAr ranges from 2.8 to 8 Å. ArKr ranges from 2.9 to 8 Å. ArKr ranges from 3 to 8 Å.

For the W4-11 database, the following molecules are taken to be multi-reference (MR): c-hooo, t-hooo, s3, cl2o, s4-c2v, of, c2, oclo, f2o, b2, fo2, cloo, foof, o3, bn, be2.

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