MultiXC-QM9: Large dataset of molecular and reaction energies from multi-level quantum chemical methods

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List of the functionals

Functional name	Details
KCIS-MODIFIED[1]	Modified version of KCIS functional
KCIS-ORIGINAL[1]	Krieger-Chen-Iafrate-Savin functional
PKZB[2]	Perdew, Kurth, Zupan and Blaha functional
VS98[3]	Voorhis-Scuseria functional
LDA(VWN)	Vosko-Wilk-Nusair[4] approximation for LDA
PW91[5–8]	The PW91 exchange and correlation.
BLYP[9–11]	Exchange Becke, Correlation Lee-Yang-Parr
BP[9, 12]	The BP86 functional
PBE[13, 14]	Perdew-Burke-Ernzerhof functional
RPBE[15]	Revised PBE by Hammer-Hansen-Norskov
REVPBE[16]	Revised PBE by Zhang-Wang
OLYP[17]	Exchange: OPTX from Henry-Cohen, correlation: PBE
FT97[18]	MetaGGA functional
BLAP3[18]	MetaGGA functional
HCTH/93[19–21]	Handy's functional refined with 93 systems
HCTH/120[19–21]	Handy's functional refined with 120 systems
HCTH/147[19–21]	Handy's functional refined with 147 systems
HCTH/407[19–21]	Handy's functional refined with 407 systems
BMTAU1[18]	MetaGGA functional
BOP[18]	MetaGGA functional

PKZBX-KCISCOR[1,2,22,23]	exchange: Perdew-Kurth-Zupan-Blahafunctional, Correlation: KCIS
VS98-X(XC)	Variation of the VS functional[3]
VS98-X-ONLY[3]	The exchange part from VS functional
BECKE00[24]	Becke's functional.
BECKE00X(XC)[24]	B Becke's functional
BECKE00-X-ONLY[24]	Becke's functional.
BECKE88X+BR89C	Becke's functional.
OLAP3	Meta-GGA functional
TPSS[25]	Tao-Perdew-Staroverov-Scuseria functional of meta-GGA type
MPBE[26]	Modified PBE functional by Adamo-Barone
OPBE[27]	GGA functional
OPERDEW[28,29]	OPERDEW
MPBEKCIS	A combination of MPBE and KCIS
MPW[30]	Modified PW by Adamo-Barone
TAU-HCTH[31]	τ-dependent functional of HCTH family
XLYP[32]	Functional XLYP
KT1[33]	Functional by Keal and Tozer
KT2[33]	Functional by Keal and Tozer
M06-L[34,35]	Minnesota functional by Yan-Truhlar
BLYP-D	BLYP functional[9,10] with Grimme's dispersion correction[36]
BP86-D	BP86 functional with Grimme's dispersion
PBE-D	PBE functional with Grimme's dispersion
TPSS-D	TPSS functional with Grimme's dispersion
B97-D	Semiempirical GGA functional[37]
REVTPSS[38]	The revised version of the TPSS functional by Perdew et. al.
PBESOL[39]	GGA functional by Perdew-Ruzsinszky-Csonka-Vydrov-Scuseria
RGE2	Regularized gradient expansion functional
SSB-D[40,41]	Dispersion corrected functional by Swart-Solà-Bickelhaupt
MVS[42]	Functional by Sun-Perdew-Ruzsinszky
MVSX	
T-MGGA[18]	
TPSSH[25,43]	TPSS functional with 10% HF exchange
B3LYP(VWN5)[44]	B3LYP by Stephens-Devlin-Chablowski-Frisch
O3LYP(VWN5)[45]	O3LYP functional

KMLYP(VWN5)[46,47]	
PBE0[48,49]	Hybrid form of PBE
B3LYP*(VWN5)[50]	Modified B3LYP functional with 15% HF exchange
BHANDH	Hybrid functional with 50% exact exchange, 50% LDA exchange, and 100% LYP correlation. Exact exchange is based on M. A. Watson et al.[47]
BHANDHLYP	Hybrid functional with 50% exact exchange, 50% Becke88 exchange, and LYP correlation. Exact exchange is based on M. A. Watson et al.[47]
B97[51]	Hybrid functional by Becke
B97-1	Hybrid functional
B97-2[52]	Hybrid functional
MPBE0KCIS[53]	
MPBE1KCIS[53]	
B1LYP(VWN5)[54]	ADF version of B1LYP by Adamo-Barone
B1PW91(VWN5)[54]	Functional by Adamo-Barone
MPW1PW[55]	Functional by Adamo-Barone
MPW1K[56]	Functional by Lynch-Fast-Harris-Truhlar
TAU-HCTH-HYBRID[57]	Hybrid functional of τ-dependent HCTH functional
X3LYP(VWN5)[58]	Functional by Xu-Goddard
OPBE0[59]	Hybrid form of OPBE
M05[60]	Minnesota M05 meta-hybrid functional
M05-2X[61]	Minnesota M05-2X meta-hybrid functional
M06[62]	Minnesota M06 meta-hybrid functional
M06-2X[63]	Minnesota M06-2X meta-hybrid functional
B3LYP-D	B3LYP with Grimme's dispersion[36] included.
GFNXTB	The semiempirical XTB2 method.

Table S1: List of Actual keys and the modified keys for the energy calculation methods. The actual keys are used in the CSV files. The modified keys are used in the SQLite3 database file. The basis set information is added at the end of the functional with underscore.

Naming of the Functional in the Database

We have changed the name of the functionals (in Table S1) if any characters other than words and numbers are present, we replaced those characters with

underscore ("_"). We used the regular expression library (*re*) in python. The basis set used (SZ, DZP or TZP) are appended at the end of the functional name with an underscore. Thus, a energy calculation method "B3LYP(VWN5)/SZ" becomes "B3LYP_VWN5__SZ

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