Supplementary Material for "Benchmark of DFT Methods on the Prediction of Bond Energies and Bond Distances of Noble-Gas Containing Molecules"

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TABLE S1. The calculated total noble-gas bond energies (TNGBEs) (in kcal/mol) by the CCSD(T)/aug-cc-pVTZ method.

	He	Ne	Ar	Kr	Xe
HNgF	-17.7		7.5	26.9	51.2
HNgCCH				9.7	32.9
FNgBO			2.9	25.0	53.1
FNgCN			-4.1	23.4	58.1
$FNgCH_3$			-1.5	17.5	42.1
FNgBNH			11.6	30.8	57.1
FNgCCH			5.7	32.7	66.0
NgBeO	5.0	5.1	12.1	15.2	18.8
NgAuF	6.3	2.5	12.4	17.9	25.2

TABLE S2. The calculated total noble-gas bond energies (TNGBEs) (in kcal/mol) by the CCSD(T)/aug-cc-pVQZ//CCSD(T)/aug-cc-pVTZ method.

	He	Ne	Ar	Kr	Xe
HNgF	-16.2		8.6	27.8	53.2
HNgCCH				9.5	33.8
FNgBO			3.0	26.1	55.3
FNgCN			-3.2	24.7	60.6
$FNgCH_3$			-0.5	18.5	44.4
FNgBNH			12.6	31.8	59.6
FNgCCH			6.9	33.0	68.9
NgBeO	5.1	5.4	11.8	14.8	19.1
NgAuF	6.4	2.5	12.9	18.5	26.9

TABLE S3. Mean unsigned error (in kcal/mol) on the TNGBE listed by different types of noble-gas molecules.[a]

Method/Basis set	6-31+G(d,p)	6-311+G(d,p)	6-311+G(2df,2pd)	aug-cc-pVDZ	aug-cc-pVTZ
			HNgF		
MP2	11.8	15.8	3.3	5.6	1.8
B3LYP	4.7	4.9	3.8	4.3	4.7
MPW1B95	4.9	5.9	2.4	2.9	2.2
MPW1PW91	6.0	7.0	3.2	3.6	2.7
B98	4.5	5.3	2.5	3.5	3.3
BMK	7.2	7.8	5.6	6.8	4.1
B3P86	4.2	3.6	6.6	6.1	7.7
M05-2X	11.4	12.4	8.9	10.9	5.9
M06-2X	11.3	12.6	8.8	10.0	5.8
B2GP-PLYP	9.3	12.0	4.4	5.6	2.3
DSD-BLYP	9.0	11.8	3.7	5.0	1.9
BLYP	11.9	9.7	13.6	13.2	14.6
MPWB95	17.3	15.1	18.9	18.6	19.8
MPWPW91	12.0	10.1	14.1	13.9	15.0
			HNgCCH		
MP2	6.3	4.4	5.7	2.7	9.2
B3LYP	4.2	3.6	2.2	2.4	2.3
MPW1B95	3.2	4.4	2.4	3.6	2.2
MPW1PW91	5.1	6.1	3.7	4.9	3.5
B98	3.1	2.2	1.9	2.3	2.0
BMK	3.8	4.4	4.1	4.8	3.9
B3P86	3.6	2.7	3.2	2.2	3.4

M05-2X	7.5	7.8	8.4	11.1	7.8
M06-2X	9.3	10.3	10.0	11.5	9.5
B2GP-PLYP	9.6	9.4	3.9	6.2	2.4
DSD-BLYP	8.9	8.4	2.3	4.8	1.5
BLYP	5.8	4.2	4.3	4.3	5.2
MPWB95	8.2	7.1	9.3	7.7	9.5
MPWPW91	5.0	3.7	6.2	4.6	6.4
			FNgBO/FNgBNH		
MP2	7.9	12.0	2.1	1.7	6.9
B3LYP	5.7	6.0	3.0	3.9	3.7
MPW1B95	5.2	6.2	2.0	2.8	2.7
MPW1PW91	6.9	9.1	3.4	4.3	3.2
B98	4.5	3.5	3.4	3.8	4.2
BMK	4.3	6.3	4.4	6.0	2.8
B3P86	4.4	3.1	4.0	4.3	4.8
M05-2X	6.7	8.6	5.0	6.5	4.6
M06-2X	12.2	14.9	10.7	11.5	7.9
B2GP-PLYP	10.0	12.9	4.2	6.5	2.5
DSD-BLYP	9.1	12.2	2.7	5.3	2.2
BLYP	8.2	5.9	10.2	9.5	11.0
MPWB95	16.8	14.8	21.4	19.2	20.5
MPWPW91	10.1	8.1	13.2	12.5	14.0
			FNgCCH/FNgCN		
MP2	6.9	3.7	16.5	13.7	22.0
B3LYP	5.9	6.6	3.3	4.3	4.2
MPW1B95	5.1	6.6	2.3	3.0	3.4
MPW1PW91	6.6	8.7	2.6	4.1	3.3

B98	4.7	4.8	3.5	3.8	4.5
BMK	6.3	8.0	2.1	4.8	1.2
B3P86	4.3	3.2	5.4	5.4	6.7
M05-2X	8.9	11.3	6.6	8.7	4.9
M06-2X	11.4	14.4	9.2	10.4	6.1
B2GP-PLYP	9.4	12.5	2.9	5.6	2.6
DSD-BLYP	7.1	10.3	2.3	3.2	3.5
BLYP	9.7	7.2	9.7	10.0	11.9
MPWB95	17.2	15.3	20.5	19.3	21.7
MPWPW91	11.4	9.6	15.2	14.0	16.4
			FNgCH3		
MP2	9.6	14.0	1.2	3.6	5.4
B3LYP	4.3	5.6	3.6	4.7	3.7
MPW1B95	3.7	5.3	2.2	3.3	2.7
MPW1PW91	6.7	8.4	4.2	4.6	3.7
B98	3.3	3.6	3.2	3.9	3.9
BMK	4.7	5.7	4.6	6.3	2.8
B3P86	3.4	2.2	3.9	4.6	4.7
M05-2X	9.8	11.2	8.3	9.6	5.7
M06-2X	10.4	12.3	9.1	9.7	6.2
B2GP-PLYP	10.7	13.5	6.3	7.6	3.2
DSD-BLYP	10.0	12.9	5.1	6.5	2.1
BLYP	9.7	8.2	11.2	10.9	11.9
MPWB95	19.9	18.4	21.5	21.1	22.3
MPWPW91	12.5	11.0	14.4	14.1	15.2
			NgBeO		
MP2	1.9	1.2	0.6	1.0	0.4

B3LYP	2.0	1.4	1.1	1.2	1.2
MPW1B95	1.7	0.9	0.9	0.8	0.8
MPW1PW91	1.6	1.1	0.8	0.7	0.8
B98	1.7	1.1	0.8	0.9	0.9
BMK	1.4	0.9	1.0	1.1	0.9
B3P86	1.5	1.0	0.8	0.7	0.8
M05-2X	2.2	0.9	1.5	1.4	1.6
M06-2X	2.2	1.0	1.6	1.4	1.6
B2GP-PLYP	1.7	1.1	0.9	0.8	0.8
DSD-BLYP	1.7	1.1	0.9	0.8	0.7
BLYP	2.1	2.0	1.5	1.4	1.5
MPWB95	1.8	1.0	0.7	0.7	0.7
MPWPW91	1.7	1.3	0.8	0.7	0.8
			NgAuF		
MP2	6.4	6.2	2.5	0.8	2.7
B3LYP	6.5	6.6	4.5	5.4	4.6
MPW1B95	5.2	5.3	2.7	4.0	2.8
MPW1PW91	5.8	5.9	3.4	4.6	3.5
B98	6.2	6.2	4.1	5.1	4.1
BMK	3.7	3.6	2.2	3.1	2.1
B3P86	5.1	5.1	2.6	3.7	2.6
M05-2X	4.2	4.0	2.4	3.2	2.3
M06-2X	5.1	5.1	4.0	4.6	3.9
B2GP-PLYP	5.9	6.4	2.0	3.4	1.9
DSD-BLYP	5.9	6.4	1.5	3.0	1.4
BLYP	7.0	7.1	5.0	5.8	5.2
MPWB95	4.9	4.9	2.4	3.6	2.5

MPWPW91	5.5	5.6	3.1	4.2	3.2

[a]The CCSD(T)/aug-cc-pVTZ and CCSD(T)/aug-cc-pVQZ methods gave MUEs of 2.4 and 1.0 kcal/mol for the HNgF group, 1.0 and 0.4 kcal/mol for the HNgCCH group, 2.5 and 1.2 kcal/mol for the FNgBO/FNgBNH group, 2.6 and 1.1 kcal/mol for the FNgCCH/FNgCN group, 2.5 and 1.0 kcal/mol for the $FNgCH_3$ group, 0.4 and 0.2 kcal/mol for the NgBeO group, and 1.0 and 0.4 kcal/mol for the NgAuF group.

[b]B2GP-PLYP and DSD-BLYP calculation was carried out using Gaussian 09 according to Ref. 74: "#p b2plyp/gen iop(3/125=0360003600,3/76=0350006500,3/78=0640006400)" for the B2GP-PLYP functional "#p b2plyp/gen iop(3/125=0400004600,3/76=0300007000,3/78=0560005600)" for the DSD-BLYP functional. The dispersion terms in DSD-BLYP were calculated according to the parameters and formulas in Ref. 74 and added to the calculated energies by Gaussian 09. The dispersion terms were neglected in the geometry optimization using the DSD-BLYP functional.

TABLE S4. Mean unsigned errors (in kcal/mol) on the TNGBE listed by different noble gases.

Method/Basis set	6-31+G(d,p)	6-311+G(d,p)	6-311+G(2df,2pd)	aug-cc-pVDZ	aug-cc-pVTZ
			Ng = He		
MP2	3.8	5.0	1.0	1.5	1.3
B3LYP	4.2	3.6	3.6	3.7	3.8
MPW1B95	1.9	1.5	1.3	1.6	1.4
MPW1PW91	1.8	1.6	1.2	1.5	1.3
B98	3.1	2.5	2.6	2.7	2.7
BMK	1.4	2.3	1.3	0.9	1.1
B3P86	4.6	4.1	4.1	4.3	4.2
M05-2X	3.4	3.7	2.1	2.9	1.5
M06-2X	3.1	3.6	2.1	2.7	1.4
B2GP-PLYP	2.2	3.4	0.7	0.7	0.7
DSD-BLYP	2.1	3.4	0.4	0.5	0.9
BLYP	8.4	7.8	7.8	7.9	7.9
MPWB95	9.5	8.8	8.7	8.9	8.8
MPWPW91	7.9	7.3	7.2	7.5	7.3
			Ng = Ne		
MP2	0.8	0.8	0.8	0.6	0.6
B3LYP	0.8	0.8	0.4	0.7	0.5
MPW1B95	0.7	0.7	0.2	0.6	0.4
MPW1PW91	0.8	1.2	0.7	0.7	0.8
B98	0.7	0.8	0.4	0.7	0.5
BMK	0.5	0.9	1.0	0.3	0.7
B3P86	0.6	1.2	0.7	0.6	0.7
M05-2X	0.8	0.1	0.8	0.9	0.9

M06-2X	1.0	0.2	0.9	1.0	0.9
B2GP-PLYP	0.6	0.6	0.4	0.2	0.1
DSD-BLYP	0.6	0.6	0.5	0.1	0.1
BLYP	0.7	1.2	0.8	0.6	0.9
MPWB95	0.4	0.6	0.1	0.3	0.3
MPWPW91	0.7	1.2	0.8	0.8	0.9
			Ng = Ar		
MP2	7.7	9.6	6.1	5.1	8.9
B3LYP	4.2	5.0	2.7	3.2	4.4
MPW1B95	6.0	7.1	1.6	1.9	2.9
MPW1PW91	7.5	8.4	1.3	1.1	1.6
B98	3.8	4.6	3.5	3.9	5.1
BMK	8.9	9.9	2.3	2.9	0.9
B3P86	1.9	2.3	5.7	6.1	7.4
M05-2X	9.6	10.0	2.1	2.2	2.1
M06-2X	12.6	13.5	5.9	5.8	2.9
B2GP-PLYP	9.0	10.7	2.1	2.9	1.2
DSD-BLYP	8.0	9.8	1.8	2.0	2.3
BLYP	9.6	8.4	12.7	13.5	14.2
MPWB95	14.7	13.7	19.0	19.2	20.0
MPWPW91	10.2	9.2	14.2	14.8	15.6
			Ng = Kr		
MP2	6.3	7.7	6.3	5.0	9.6
B3LYP	2.6	2.9	1.5	1.5	1.9
MPW1B95	2.3	3.4	1.1	1.5	1.3
MPW1PW91	2.2	4.9	2.0	3.1	1.7
B98	3.3	1.9	2.2	1.6	2.8

BMK	3.8	6.0	2.6	4.9	1.9
B3P86	5.7	2.5	4.6	3.6	5.2
M05-2X	6.2	8.8	5.5	7.2	3.1
M06-2X	7.6	10.6	7.4	8.3	5.2
B2GP-PLYP	5.1	8.9	2.7	4.9	1.4
DSD-BLYP	4.2	8.1	1.8	3.6	1.6
BLYP	11.6	8.2	9.2	9.3	10.4
MPWB95	17.4	14.1	16.2	15.1	16.3
MPWPW91	13.3	10.1	11.6	11.0	12.2
			Ng = Xe		
MP2	9.8	9.9	5.0	5.4	7.5
B3LYP	8.9	9.0	5.4	7.2	5.2
MPW1B95	6.3	7.0	4.2	5.9	4.0
MPW1PW91	9.5	10.0	6.3	8.1	6.2
B98	6.5	6.7	3.7	5.7	3.5
BMK	3.3	2.6	5.7	7.9	4.7
B3P86	4.2	4.5	2.0	3.0	2.0
M05-2X	7.9	8.0	10.3	12.9	9.1
M06-2X	10.3	11.0	12.0	13.6	10.7
B2GP-PLYP	13.1	13.3	6.5	9.0	4.8
DSD-BLYP	12.3	12.5	4.9	7.6	2.9
BLYP	3.6	3.2	4.4	3.4	4.8
MPWB95	8.7	8.5	11.3	9.8	11.2
MPWPW91	3.9	3.6	6.8	5.5	6.9

[a]The CCSD(T)/aug-cc-pVTZ and CCSD(T)/aug-cc-pVQZ methods gave MUEs of 1.0 and 0.4 kcal/mol for the He group, 0.2 and 0.1 kcal/mol for the Ne group, 1.5 and 0.7 kcal/mol for the Ar group, 1.3 and 0.6 kcal/mol for the Kr group, 3.3 and 1.4 kcal/mol for the Xe group.

TABLE S5. Mean unsigned errors (in Å) on the NGBD listed by different types of noble-gas bonds.

	6-31+G(d,p)	6-311+G(d,p)	6-311+G(2df,2pd)	aug-cc-pVDZ	aug-cc-pVTZ
			H–Ng		
MP2	0.010	0.005	0.016	0.007	0.020
B3LYP	0.030	0.032	0.024	0.027	0.021
MPW1B95	0.016	0.020	0.014	0.016	0.013
MPW1PW91	0.019	0.024	0.016	0.019	0.014
B98	0.026	0.031	0.021	0.024	0.019
BMK	0.023	0.026	0.019	0.021	0.018
B3P86	0.024	0.029	0.020	0.023	0.018
M05-2X	0.011	0.014	0.018	0.015	0.020
M06-2X	0.013	0.016	0.017	0.015	0.020
B2GP-PLYP	0.010	0.017	0.011	0.012	0.010
DSD-BLYP	0.011	0.016	0.010	0.011	0.009
BLYP	0.078	0.075	0.060	0.067	0.055
MPWB95	0.074	0.071	0.054	0.060	0.050
MPWPW91	0.066	0.063	0.049	0.054	0.045
			Be–Ng		
MP2	0.020	0.017	0.004	0.044	0.002
B3LYP	0.012	0.018	0.012	0.016	0.018
MPW1B95	0.009	0.010	0.004	0.013	0.008
MPW1PW91	0.008	0.011	0.007	0.016	0.007
B98	0.016	0.021	0.012	0.026	0.007
BMK	0.021	0.023	0.021	0.007	0.029
B3P86	0.009	0.010	0.007	0.010	0.011
M05-2X	0.022	0.014	0.014	0.024	0.018

M06-2X	0.021	0.013	0.019	0.023	0.023
B2GP-PLYP	0.015	0.014	0.013	0.021	0.014
DSD-BLYP	0.016	0.015	0.011	0.024	0.013
BLYP	0.024	0.033	0.026	0.031	0.021
MPWB95	0.023	0.028	0.024	0.029	0.018
MPWPW91	0.021	0.025	0.018	0.029	0.012
			B–Ng		
MP2	0.011	0.008	0.016	0.004	0.018
B3LYP	0.051	0.049	0.031	0.040	0.028
MPW1B95	0.016	0.012	0.004	0.004	0.006
MPW1PW91	0.028	0.024	0.009	0.015	0.008
B98	0.051	0.047	0.026	0.034	0.024
BMK	0.028	0.029	0.020	0.014	0.020
B3P86	0.037	0.032	0.016	0.023	0.013
M05-2X	0.008	0.003	0.009	0.005	0.012
M06-2X	0.007	0.005	0.010	0.006	0.012
B2GP-PLYP	0.023	0.021	0.003	0.016	0.008
DSD-BLYP	0.023	0.022	0.003	0.017	0.009
BLYP	0.113	0.112	0.087	0.096	0.082
MPWB95	0.091	0.088	0.063	0.069	0.059
MPWPW91	0.089	0.084	0.062	0.068	0.058
			C–Ng		
MP2	0.021	0.022	0.026	0.018	0.032
B3LYP	0.037	0.040	0.022	0.033	0.024
MPW1B95	0.011	0.011	0.030	0.021	0.032
MPW1PW91	0.011	0.012	0.021	0.018	0.024
B98	0.029	0.028	0.015	0.023	0.017

BMK	0.019	0.021	0.024	0.022	0.027
B3P86	0.017	0.016	0.017	0.020	0.020
M05-2X	0.014	0.018	0.028	0.026	0.032
M06-2X	0.015	0.018	0.030	0.025	0.034
B2GP-PLYP	0.020	0.022	0.011	0.015	0.017
DSD-BLYP	0.025	0.027	0.010	0.014	0.017
BLYP	0.104	0.111	0.079	0.089	0.073
MPWB95	0.072	0.076	0.044	0.054	0.039
MPWPW91	0.065	0.068	0.038	0.048	0.035
			F–Ng		
MP2	0.032	0.045	0.011	0.017	0.011
B3LYP	0.043	0.056	0.022	0.025	0.014
MPW1B95	0.017	0.030	0.005	0.007	0.014
MPW1PW91	0.018	0.031	0.005	0.009	0.013
B98	0.032	0.045	0.010	0.015	0.006
BMK	0.030	0.043	0.014	0.013	0.008
B3P86	0.020	0.033	0.005	0.011	0.012
M05-2X	0.017	0.027	0.008	0.009	0.011
M06-2X	0.014	0.023	0.008	0.007	0.013
B2GP-PLYP	0.035	0.049	0.009	0.018	0.004
DSD-BLYP	0.037	0.050	0.008	0.019	0.005
BLYP	0.080	0.093	0.058	0.060	0.048
MPWB95	0.059	0.072	0.036	0.038	0.025
MPWPW91	0.052	0.065	0.028	0.031	0.019
			Au–Ng		
MP2	0.153	0.158	0.060	0.018	0.066
B3LYP	0.161	0.166	0.067	0.088	0.060

MPW1B95	0.113	0.156	0.025	0.049	0.022
MPW1PW91	0.132	0.133	0.030	0.053	0.024
B98	0.172	0.172	0.061	0.086	0.052
BMK	0.085	0.084	0.033	0.055	0.036
B3P86	0.104	0.106	0.010	0.032	0.008
M05-2X	0.113	0.120	0.053	0.077	0.051
M06-2X	0.164	0.168	0.105	0.127	0.103
B2GP-PLYP	0.153	0.157	0.011	0.043	0.006
DSD-BLYP	0.153	0.157	0.003	0.035	0.005
BLYP	0.192	0.197	0.097	0.116	0.089
MPWB95	0.128	0.127	0.043	0.063	0.038
MPWPW91	0.144	0.143	0.042	0.063	0.035

TABLE S6. Mean unsigned errors (in Å) on the NGBD listed by different noble gases.

	6-31+G(d,p)	6-311+G(d,p)	6-311+G(2df,2pd)	aug-cc-pVDZ	aug-cc-pVTZ
			Ng = He		
MP2	0.058	0.045	0.019	0.028	0.020
B3LYP	0.058	0.059	0.028	0.032	0.025
MPW1B95	0.049	0.041	0.009	0.025	0.009
MPW1PW91	0.052	0.042	0.013	0.028	0.010
B98	0.068	0.060	0.022	0.039	0.019
BMK	0.034	0.039	0.021	0.022	0.025
B3P86	0.044	0.038	0.012	0.023	0.010
M05-2X	0.053	0.042	0.019	0.039	0.022
M06-2X	0.054	0.054	0.040	0.047	0.040
B2GP-PLYP	0.053	0.052	0.010	0.022	0.011
DSD-BLYP	0.051	0.067	0.007	0.015	0.015
BLYP	0.088	0.085	0.051	0.057	0.048
MPWB95	0.082	0.075	0.042	0.054	0.037
MPWPW91	0.078	0.069	0.034	0.049	0.031
			Ng = Ne		
MP2	0.084	0.146	0.032	0.044	0.041
B3LYP	0.079	0.107	0.034	0.035	0.037
MPW1B95	0.049	0.189	0.032	0.027	0.039
MPW1PW91	0.080	0.126	0.042	0.044	0.035
B98	0.095	0.138	0.065	0.071	0.043
BMK	0.025	0.015	0.040	0.032	0.066
B3P86	0.045	0.083	0.005	0.005	0.008
M05-2X	0.017	0.043	0.020	0.023	0.034

M06-2X	0.038	0.036	0.018	0.019	0.027
B2GP-PLYP	0.077	0.108	0.011	0.009	0.013
DSD-BLYP	0.033	0.031	0.008	0.019	0.007
BLYP	0.096	0.137	0.068	0.066	0.050
MPWB95	0.057	0.094	0.055	0.043	0.046
MPWPW91	0.093	0.135	0.058	0.056	0.041
			Ng = Ar		
MP2	0.048	0.060	0.019	0.019	0.028
B3LYP	0.063	0.077	0.027	0.028	0.020
MPW1B95	0.033	0.044	0.018	0.021	0.026
MPW1PW91	0.035	0.045	0.018	0.021	0.024
B98	0.053	0.066	0.019	0.021	0.017
BMK	0.038	0.050	0.030	0.026	0.029
B3P86	0.038	0.049	0.016	0.019	0.024
M05-2X	0.035	0.044	0.028	0.026	0.034
M06-2X	0.039	0.048	0.033	0.031	0.040
B2GP-PLYP	0.048	0.063	0.010	0.016	0.015
DSD-BLYP	0.051	0.067	0.007	0.015	0.015
BLYP	0.130	0.144	0.078	0.077	0.061
MPWB95	0.102	0.115	0.050	0.050	0.033
MPWPW91	0.091	0.104	0.040	0.040	0.027
			Ng = Kr		
MP2	0.029	0.027	0.019	0.014	0.021
B3LYP	0.042	0.042	0.025	0.033	0.022
MPW1B95	0.017	0.018	0.013	0.011	0.016
MPW1PW91	0.020	0.019	0.011	0.012	0.013
B98	0.034	0.032	0.015	0.023	0.012

BMK	0.024	0.030	0.019	0.015	0.015
B3P86	0.023	0.020	0.010	0.013	0.013
M05-2X	0.020	0.022	0.017	0.016	0.017
M06-2X	0.022	0.025	0.023	0.021	0.025
B2GP-PLYP	0.030	0.031	0.009	0.020	0.007
DSD-BLYP	0.033	0.031	0.008	0.019	0.007
BLYP	0.084	0.084	0.065	0.074	0.060
MPWB95	0.059	0.057	0.039	0.048	0.035
MPWPW91	0.055	0.052	0.034	0.043	0.030
			Ng = Xe		
MP2	0.021	0.023	0.018	0.014	0.015
B3LYP	0.040	0.045	0.028	0.040	0.026
MPW1B95	0.013	0.017	0.007	0.010	0.010
MPW1PW91	0.018	0.022	0.007	0.016	0.009
B98	0.036	0.040	0.017	0.029	0.017
BMK	0.032	0.035	0.009	0.015	0.009
B3P86	0.020	0.026	0.009	0.021	0.009
M05-2X	0.014	0.015	0.011	0.016	0.012
M06-2X	0.019	0.019	0.015	0.018	0.016
B2GP-PLYP	0.025	0.029	0.009	0.023	0.006
DSD-BLYP	0.026	0.030	0.008	0.022	0.005
BLYP	0.075	0.080	0.062	0.075	0.060
MPWB95	0.053	0.058	0.037	0.049	0.035
MPWPW91	0.050	0.055	0.035	0.047	0.033