Extrapolating DFT towards the complete basis set limit: Lessons from the PBE family of functionals

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Supplementary Material

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Additional supplemental files and archives in computer-readable form are available on Zenodo, see DOI: 10.5281/zenodo.4783007. An executable version of this archive is available on Binder.

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Table S1: List of methods used with the diet100 variant of the GMTKN55 database. References correspond to functionals and parametrizations of dispersion corrections.

Method name	**DFA type**	**Disp. type**	**Reference**
BLYP-D3(BJ)	GGA	D3(BJ)	1;2;3
PBE-D3(BJ)	GGA	D3(BJ)	4;3
revPBE-D3(BJ)	GGA	D3(BJ)	5;4;3
B97-D3(BJ)	GGA	D3(BJ)	6;3
SCAN-D3(BJ)	mGGA	D3(BJ)	7;8
M06L-D3	mGGA	D3(0)	9;10
B97M-V	mGGA	VV10	11
B97M-D3(BJ)	mGGA	D3(BJ)	11;12
B3LYP-D3(BJ)	single hyb.	D3(BJ)	13;14;3
ωB97X-V	single hyb.	VV10	15
M052X-D3	single hyb.	D3(0)	16;10
dlDF+D10	single hyb.	DAS2010	17;18
DSD-BLYP-D3(BJ)	double hyb.	D3(BJ)	19
B2PLYP-D3(BJ)	double hyb.	D3(BJ)	20;10
PWPB95-NL	double hyb.	VV10	21;22;23
PBE0DH-D3(BJ)	double hyb.	D3(BJ)	24;25

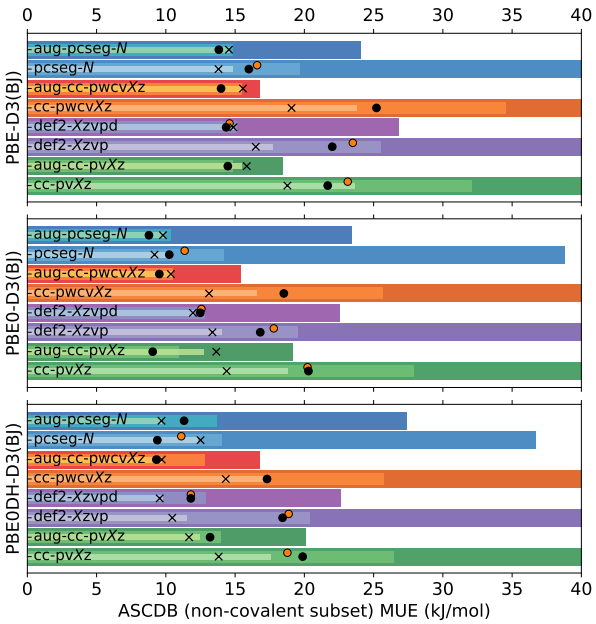

Figure S1: The total of the mean unsigned errors in the non-covalent subset of the ASCDB database. Calculations with 2-, 3-, and 4-ζ basis sets shown as bars. Results from the [2,3]-ζ extrapolation (•) and [3,4]-ζ extrapolation (×) from current work compared to previous [2,3]-ζ results (•), where available.

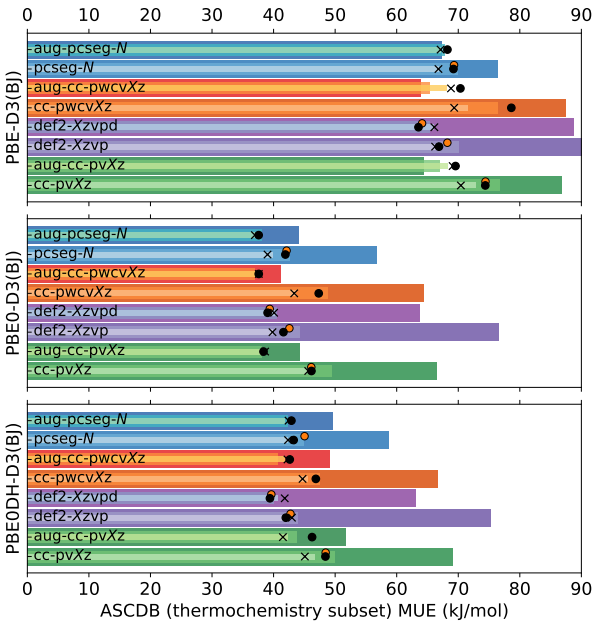

Figure S2: The total of the mean unsigned errors in the thermochemistry subset of the ASCDB database. Bars and symbols as in Fig. S1.

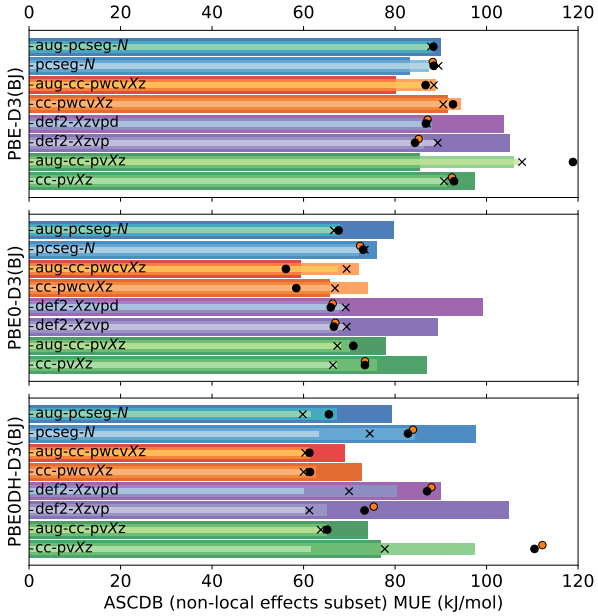

Figure S3: The total of the mean unsigned errors in the non-local subset of the ASCDB database. Bars and symbols as in Fig. S1.

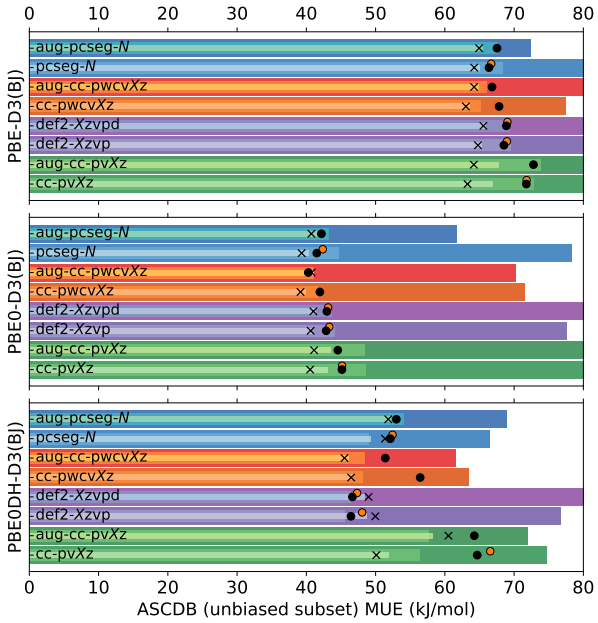

Figure S4: The total of the mean unsigned errors in the unbiased calculations subset of the ASCDB database. Bars and symbols as in Fig. S1.

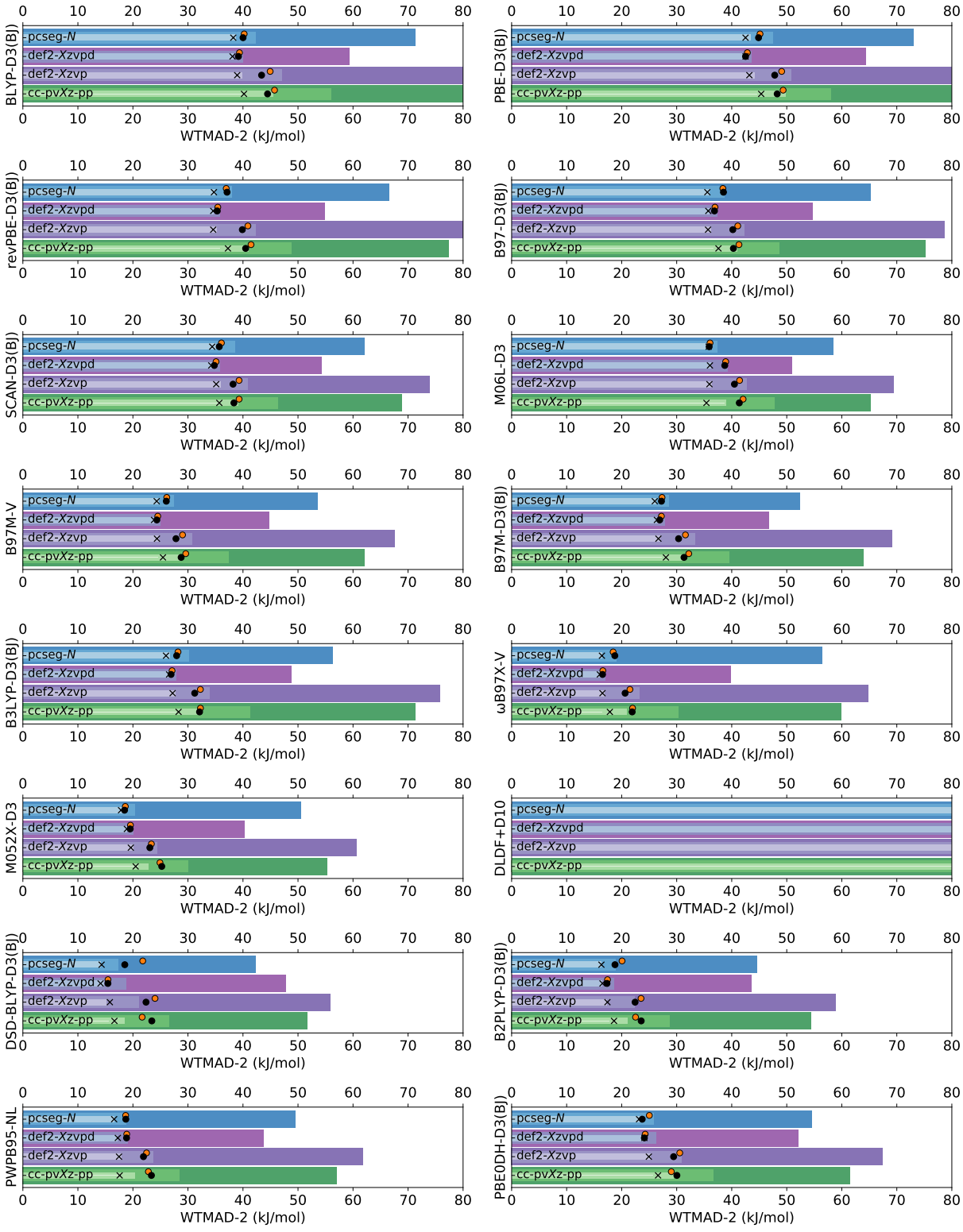

Figure S5: The WTMAD-2 measures of the diet100 subset of the GMTKN55 database. Bars and symbols as in Fig. S1.

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