

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

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Supplementary Material

## Table of contents

- |   |       |
|---|-------|
| 1. Figures of results for the subsets of the ASCDB database                                 | p. S2 |
| 2. Figures of results for all methods used with the diet100 subsets of the GMTKN55 database | p. S6 |

Additional supplemental files and archives in computer-readable form are available on Zenodo, see DOI: [10.5281/zenodo.4783007](https://doi.org/10.5281/zenodo.4783007). An executable version of this archive is available on [Binder](#).

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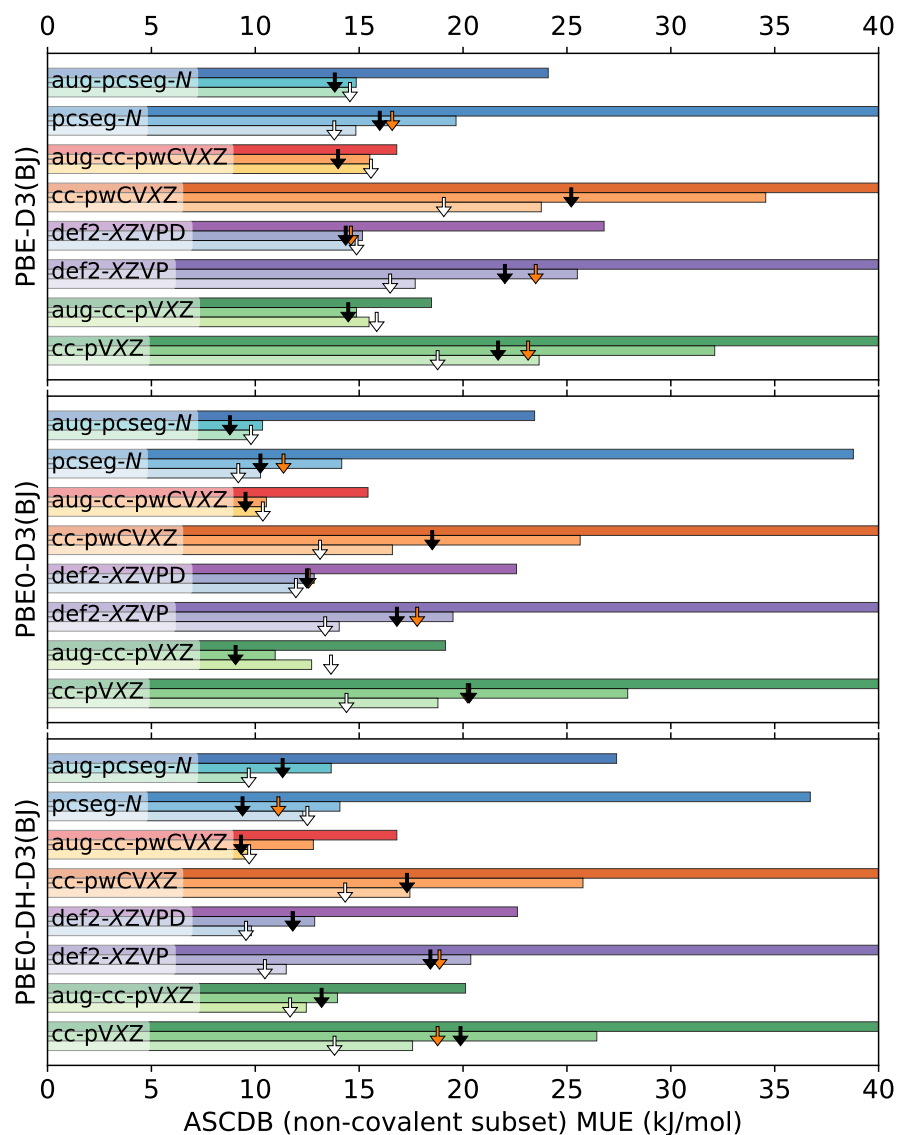


Figure S1: The total of the mean unsigned errors in the non-covalent subset of the ASCDB database. Calculations with 2-, 3-, and 4- $\zeta$  basis sets shown as horizontal bars in ascending order. Results from the [2,3]- $\zeta$  and [3,4]- $\zeta$  extrapolations from current work are indicated by the black and white arrows, respectively. Comparison with previous [2,3]- $\zeta$  results (orange arrow) shown where available.

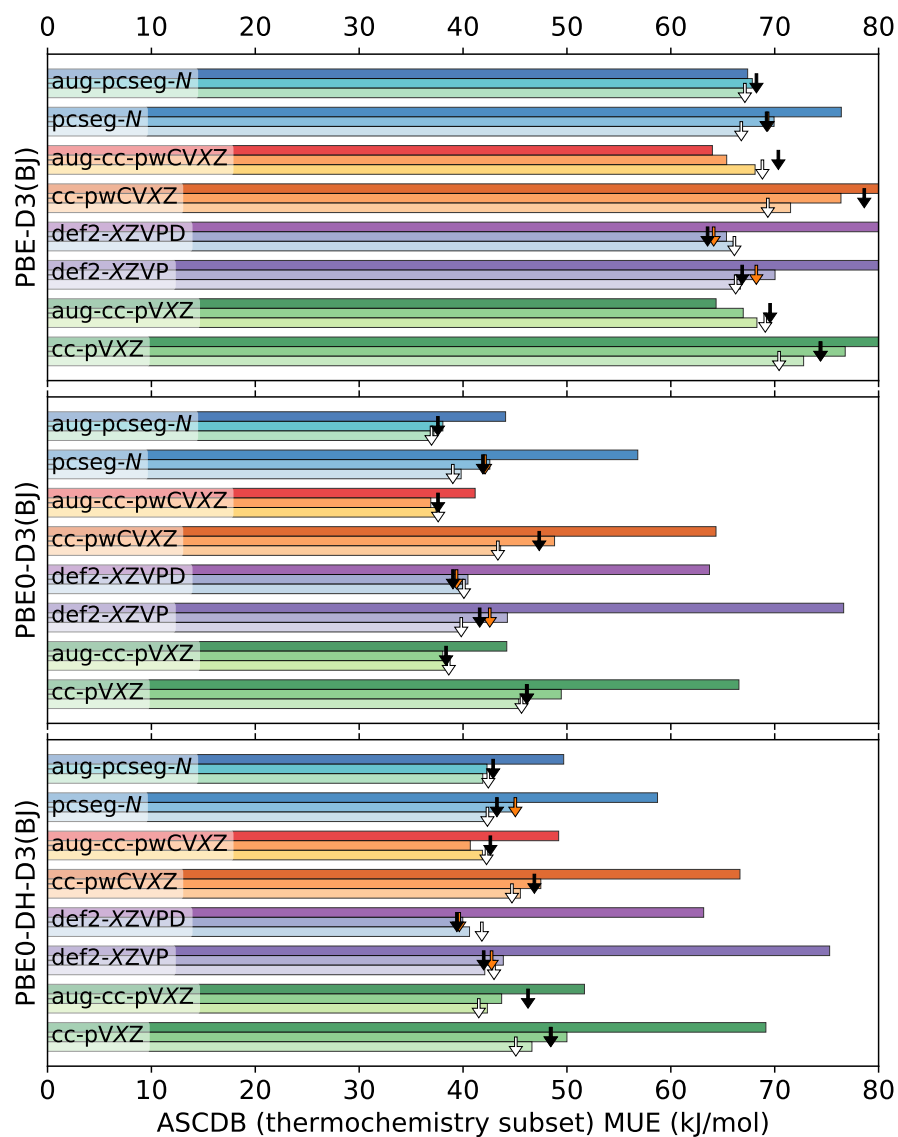


Figure S2: The total of the mean unsigned errors in the thermochemistry subset of the ASCDB database. Bars and symbols as in Fig. S1.

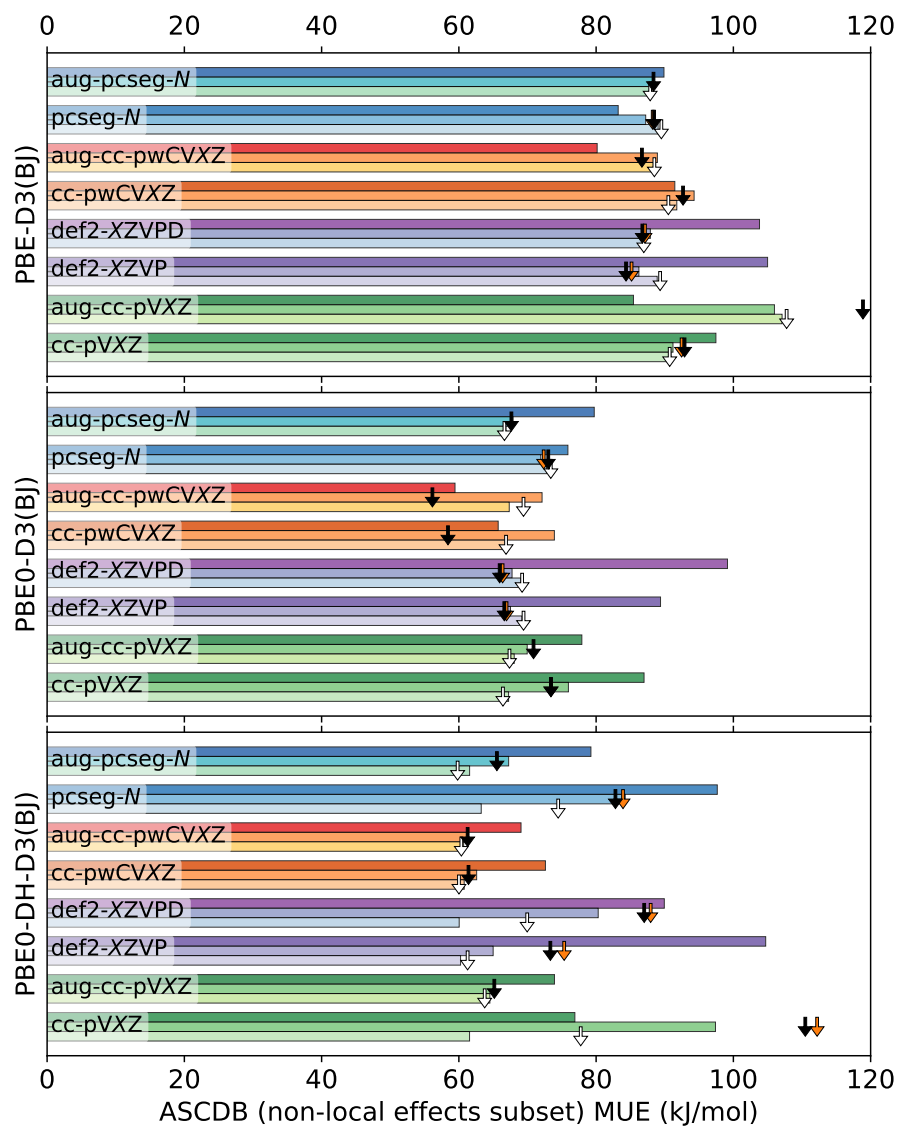


Figure S3: The total of the mean unsigned errors in the non-local subset of the ASCDB database. Bars and symbols as in Fig. S1.

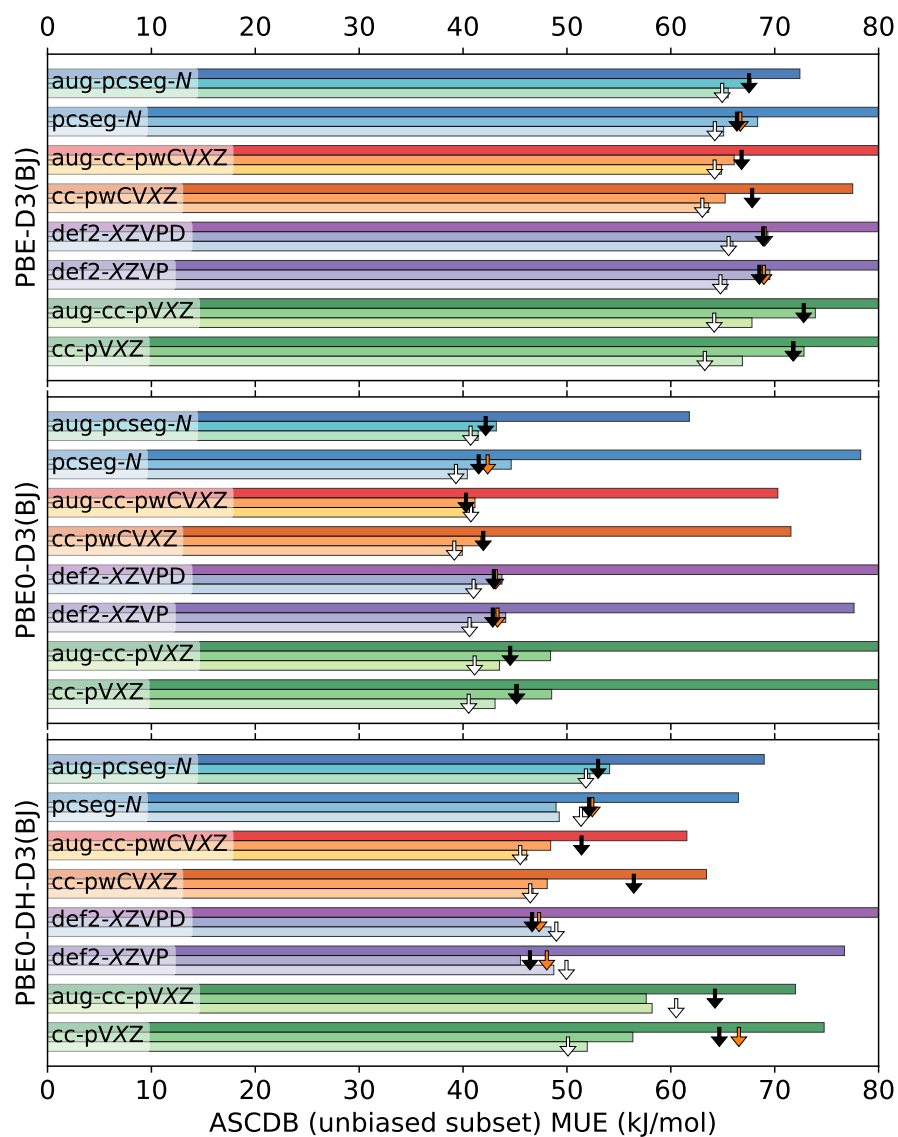


Figure S4: The total of the mean unsigned errors in the unbiased calculations subset of the ASCDB database. Bars and symbols as in Fig. S1.

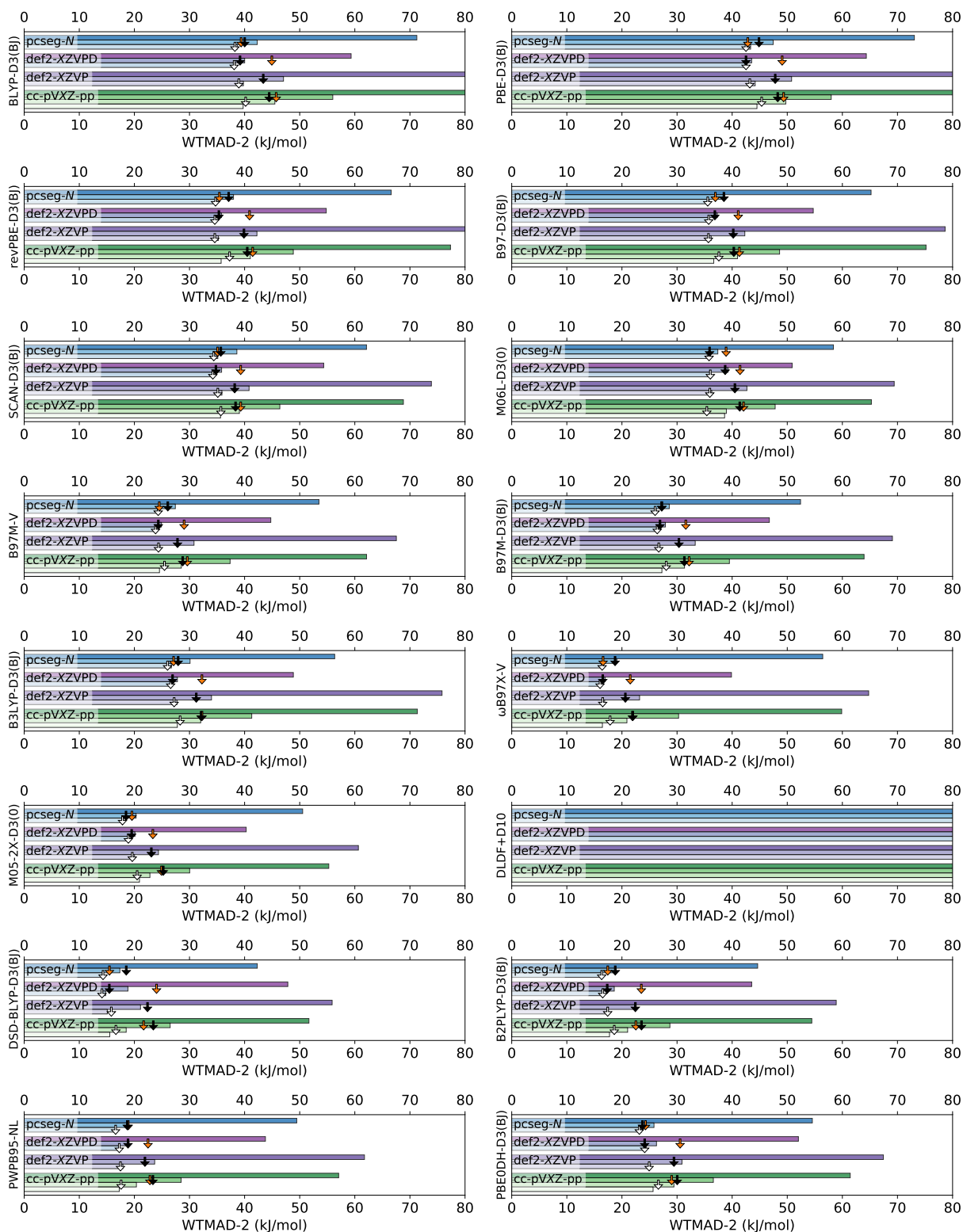


Figure S5: The WTMAD-2 measures of the diet100 subset of the GMTKN55 database. Bars and symbols as in Fig. S1. For the cc-pVXZ-pp basis sets, data from 2-, 3-, 4-, and 5- $\zeta$  basis sets shown.