



Cite this: *Phys. Chem. Chem. Phys.*, 2018, 20, 4606

Correction: General optimization procedure towards the design of a new family of minimal parameter spin-component-scaled double-hybrid density functional theory†

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DOI: 10.1039/c8cp90025f

rsc.li/pccp

Correction for 'General optimization procedure towards the design of a new family of minimal parameter spin-component-scaled double-hybrid density functional theory' by Loïc M. Roch and Kim K. Baldridge, *Phys. Chem. Chem. Phys.*, 2017, **19**, 26191–26200.

In eqn (1) and (3), C_X should be defined as the coefficient scaling the exact HF exchange, and, thus, $(1 - C_X)$ as the coefficient scaling the approximate GGA exchange. Consequently, eqn (1) should read:

$$E_{XC}^{DSD-DFT} = (1 - C_X)E_X^{GGA} + C_X E_X^{HF} + C_C E_C^{GGA} + C_O E_O^{MP2} + C_S E_S^{MP2} + S_6 E_D \quad (1)$$

and eqn (3) should read:

$$E_{XC}^{mSD-DFT} = (1 - C_X)E_X^{GGA} + C_X E_X^{HF} + C_C E_C^{GGA} + (1 - C_C)E_{(2)}^{SCS-MP2} \quad (3)$$

Note that C_{HF} , which is not formally introduced although used in the manuscript, in Fig. 2–4 and in the ESI, scales the HF exchange of the mSD-DF. As such, C_{HF} is equivalent to C_X .

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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† Electronic supplementary information (ESI) available: Basis set considerations, tabulation of interaction energies of the complexes included in the training set, grid refinement and scaled RMSD. See DOI: 10.1039/c8cp90025f

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