PCCP



View Article Online

CORRECTION

Check for updates

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[†]

Loïc M. Roch‡^{ab} and Kim K. Baldridge§*^{ab}

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:

$$E_{\rm XC}^{\rm DSD-DFT} = (1 - C_{\rm X})E_{\rm X}^{\rm GGA} + C_{\rm X}E_{\rm X}^{\rm HF} + C_{\rm C}E_{\rm C}^{\rm GGA} + C_{\rm O}E_{\rm O}^{\rm MP2} + C_{\rm S}E_{\rm S}^{\rm MP2} + S_{\rm 6}E_{\rm D}$$
(1)

and eqn (3) should read:

$$E_{\rm XC}^{\rm mSD-DFT} = (1 - C_{\rm X})E_{\rm X}^{\rm GGA} + C_{\rm X}E_{\rm X}^{\rm HF} + C_{\rm C}E_{\rm C}^{\rm GGA} + (1 - C_{\rm C})E_{(2)}^{\rm SCS-MP2}$$
(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.

^a Department of Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland. E-mail: kimb@tju.edu.cn

^b Health Sciences Platform, University of Tianjin, 92 Weijin Road, Nankai District, Tianjin-3000072, P. R. China

[†] 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

[‡] Present address: Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, MA, USA.

[§] Present address: Health Sciences Platform, Tianjin University, 92 Weijing Road, Nankai District, Tianjin-3000072, P. R. China.