



Cite this: *Phys. Chem. Chem. Phys.*,
2022, 24, 19975

Correction: Computational approaches for XANES, VtC-XES, and RIXS using linear-response time-dependent density functional theory based methods

Daniel R. Nascimento^{*a} and Niranjana Govind^{*b}

DOI: 10.1039/d2cp90142k

rsc.li/pccp

Correction for 'Computational approaches for XANES, VtC-XES, and RIXS using linear-response time-dependent density functional theory based methods' by Daniel R. Nascimento *et al.*, *Phys. Chem. Chem. Phys.*, 2022, 24, 14680–14691, <https://doi.org/10.1039/D2CP01132H>.

The authors would like to include 3 additional references in the last paragraph of column 1 on page 14686. The original sentence reads as follows:

"This simplified approach is equivalent to the pseudo-wavefunction formulation of LR-TDDFT (PWF-TDDFT) proposed originally in the context of derivative couplings between Hartree-Fock excited states¹⁷⁶ and spin-flip TDDFT states,¹⁷⁷ then generalized to LR-TDDFT states.^{178,179}"

This should be changed to the following text, where the new references are added as 188, 189 and 190:

"This simplified approach is equivalent to the pseudo-wavefunction formulation of LR-TDDFT (PWF-TDDFT) proposed originally in the context of derivative couplings between Hartree-Fock excited states¹⁷⁶ and spin-flip TDDFT states,¹⁷⁷ then generalized to LR-TDDFT states.^{178,179,188–190}"

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

References

- 188 Z. Li and W. Liu, First-order nonadiabatic coupling matrix elements between excited states: A Lagrangian formulation at the CIS, RPA, TD-HF, and TD-DFT levels, *J. Chem. Phys.*, 2014, **141**(1), 014110.
- 189 Z. Li, B. Suo and W. Liu, First order nonadiabatic coupling matrix elements between excited states: Implementation and application at the TD-DFT and pp-TDA levels, *J. Chem. Phys.*, 2014, **141**(24), 244105.
- 190 Z. Wang, C. Wu and W. Liu, NAC-TDDFT: Time-dependent density functional theory for nonadiabatic couplings, *Acc. Chem. Res.*, 2021, **54**(17), 3288–3297.

^a Department of Chemistry, The University of Memphis, Memphis, TN, 38152, USA. E-mail: daniel.nascimento@memphis.edu

^b Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, Washington 99352, USA. E-mail: niri.govind@pnnl.gov

