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

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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


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