CORRECTION

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Correction: Benchmarking DFT-based excited-state methods for intermolecular charge-transfer excitations

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Correction for 'Benchmarking DFT-based excited-state methods for intermolecular charge-transfer excitations' by Nicola Bogo *et al.*, *Phys. Chem. Chem. Phys.*, 2024, **26**, 21575–21588, https://doi.org/10.1039/D4CP01866D.

In our article "*Benchmarking DFT-based excited-state methods for intermolecular charge-transfer excitations*", we included several reference calculations with the EOM-CCSD(fT) method. Due to an error in our output parsing routine, the effect of the triples correction was omitted from these results, resulting in a rather constant redshift of the corresponding reference excitation energies. Incorporating the triples correction accordingly leads to a blueshift of the excitation energies compared to the published data. This directly affects the following in the original publication:

- Panel A of Fig. 2
- Fig. 3
- Table 1

Since we discuss these data in the manuscript, several error metrics discussed there are also incorrect and need to be adapted according to the data provided in this erratum. We emphasize that the conclusions of our manuscript are unchanged. As stated in the original article, orbital-optimized DFT yields the lowest absolute errors and, importantly, a very small variance of the results compared to the now-corrected EOM-CCSD(fT) reference values.

We present here the corrected Fig. 2 and 3 (displayed herein as Fig. 1 and 2, respectively) and Table 1, and additionally provide Fig. 3, which is similar to Fig. 3 in the original article but includes only reference data obtained with the EOM-CCSD(fT) method, yielding a more faithful estimate of the error statistics.

In addition to these numerical errors arising from a rather constant increased offset of the excitation energies, we correct our discussion on the pleasing performance of the TDA data, particularly for the tetrafluoroethylene–ethylene dimer, since the results of this method are much less favourable in light of the correct reference energies.

The corrected data has been deposited in a Zenodo repository and can be accessed under https://doi.org/10.5281/zenodo.18388464.

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

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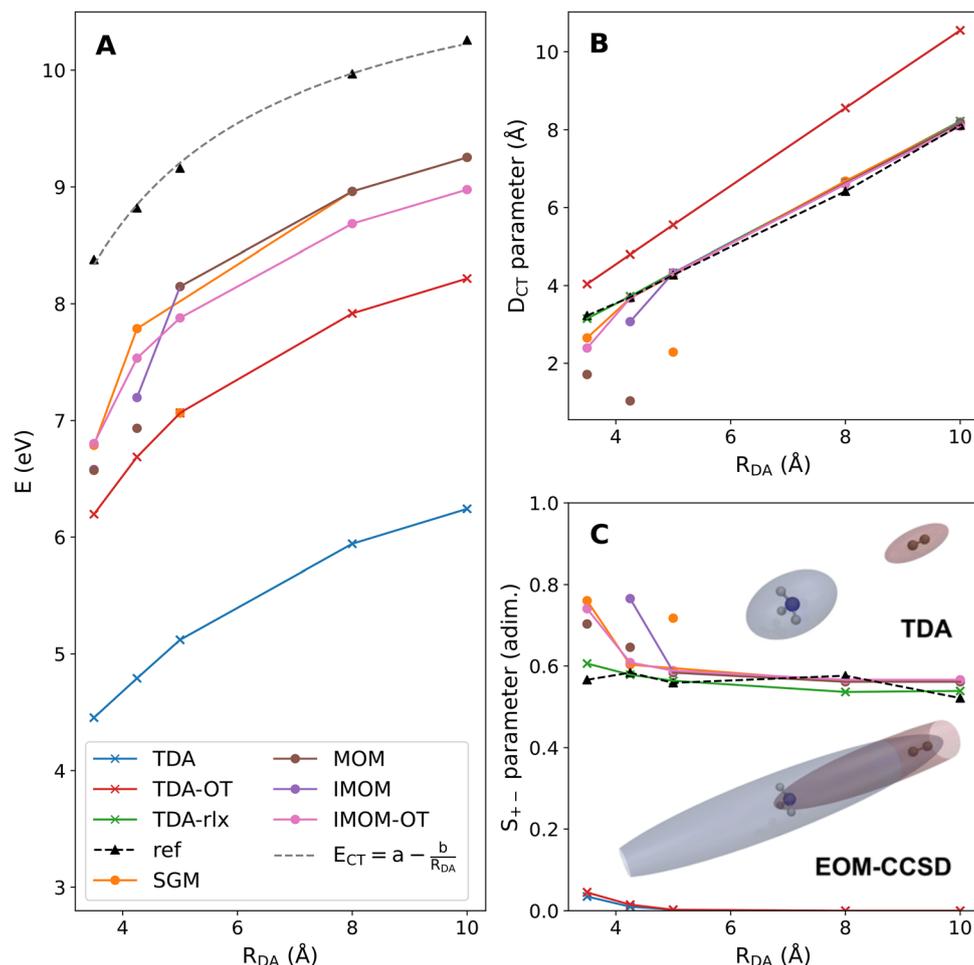*Phys. Chem. Chem. Phys.*, 2026, **28**, 6127–6129 | **6127**

Fig. 1   [Correction of Fig. 2 in the published paper] – Panel A: CT excitation energy belonging to the lowest-lying CT state of the ammonia–fluorine dimer vs. donor–acceptor separation distance (Å) computed with the EOM-CCSD(fT) (ref.), TDA, optimally tuned TDA (TDA-OT), IMOM, MOM, and SGM methods, respectively. Data points characterised by $D_{CT} > \frac{1}{2} R_{DA}$ are connected with solid lines. The reference data is fitted to Mulliken's equation for the CT excitation energy (eqn (14)), using the 2-parameter expression $E_{CT} = a - \frac{b}{R_{DA}}$, where a = $IP_D - EA_A$ and b is a system-specific parameter with unit of energy times distance. Panel B: D_{CT} parameter (Å) computed on the lowest-lying CT state vs. donor–acceptor separation distance (Å) computed with the EOM-CCSD(fT) (ref.), TDA, optimally tuned TDA (TDA-OT), relaxed TDA (TDA-rlx), IMOM, MOM, and SGM densities. Panel C: S_{+-} diagnostic computed for the lowest-lying CT state vs. donor–acceptor separation distance (Å). Inset: Isosurface plot of the normalized C_+ and C_- ellipsoids produced by Multiwfn, using TDA and EOM-CCSD densities at 10 Å separation. The isovalue is ±0.0001 for C_+ and C_-.
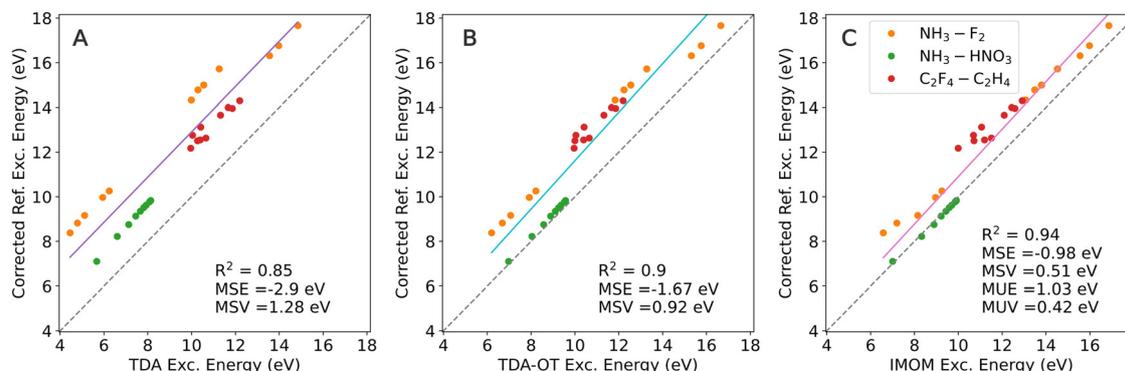

Fig. 2   [Correction of Fig. 3 in the published paper] – Excitation energy to the low-lying ICT states in the R_{DA}-dataset. The data points belonging to the beryllium–fluorine dimer were excluded from this plot. Dashed grey line: target trend, where the reference and the DFT energy are the same. Solid lines: linear fit. The color-coding highlights data points belonging to the molecular dimers in the dataset.

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Table 1 *[Correction of Table 1 in the published paper]* – Reference method, mean signed error (MSE) and mean signed variance (MSV) on the ICT excitation energy for each dimer system scan investigated, using the various DFT-based excited-state electronic structure methods, the LRC-ωPBE XCF and the def2-TZVP basis. Entries in the row *All* correspond to a linear fit of all datapoints combined in a single dataset. The rightmost column lists the ICT states which are included in the scan, and the number of data points after the selection based on the D_{CT} descriptor in parentheses (see Section 5). All values reported in eV unit

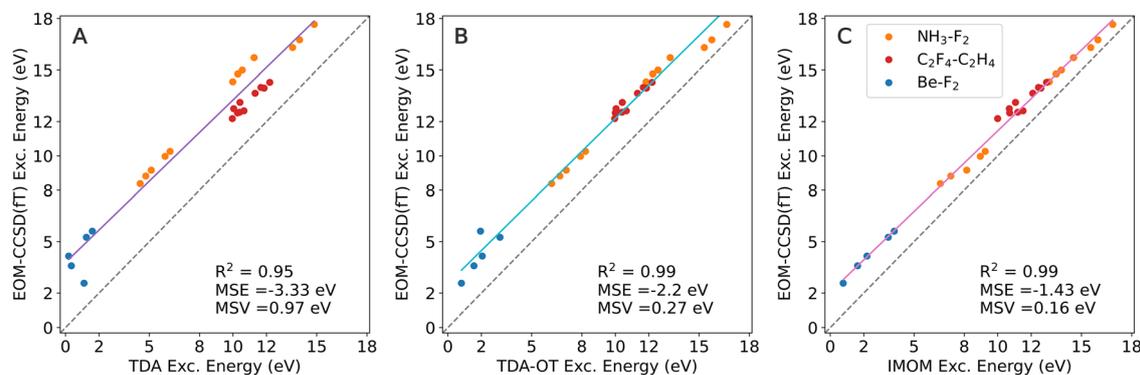| Dimer	Ref. method	TDA		TDA-OT		IMOM		Nr. ICTs
		MSE	MSV	MSE	MSV	MSE	MSV	
B–F_2	EOM-CCSD(fT)	−3.34	1.20	−2.35	0.57	−1.86	0.01	1(5)
NH_3–F_2	EOM-CCSD(fT)	−3.99	0.40	−2.08	0.32	−1.17	0.08	4(17)
NH_3–HNO_3	SA2-MS-CAS(2,2)PT2	−1.64	0.01	−0.22	0.00	0.07	0.00	1(9)
C_2F_4–C_2H_4	EOM-CCSD(fT)	−2.28	0.06	−2.31	0.07	−1.64	0.13	3(15)
All	Both	−2.95	1.26	−1.75	0.91	−1.09	0.53	9(45)
$D_{CT} > 0.5R_{DA}$	Both	−2.90	1.28	−1.67	0.92	−0.98	0.51	8(36)
Same ref. method	EOM-CCSD(fT)	−3.33	0.97	−2.17	0.23	−1.35	0.15	7(27)

Fig. 3 *[Additional new figure similar to the previous Fig. 3 but including only EOM-CCSD(f T) reference data]* – Excitation energy to the low-lying ICT states computed with the EOM-CCSD(fT) method. Dashed grey line: target trend, where the reference and the DFT energy are the same. Solid lines: linear fit. The color-coding highlights data points belonging to the molecular dimers in the dataset.

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