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Erratum: "Non-orthogonal configuration interaction with single substitutions for the calculation of core-excited states" [J. Chem. Phys. 149, 044116 (2018)]

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In our recent publication[1], we incorrectly stated some of the CIS and TDDFT k-edge excitations. Specifically the errors were in the CIS k-edge for all molecules except C2N2 and C2H6 and the TDDFT k-edge for only C2H2, N2, CO2 O, F2, and C2H2, all of which are shown in Table II of the original paper. A corrected version of that table can be found below. This changes our results slightly in that the RMSEs of the CIS and the TDDFT results are slightly reduced, but it does not change the primary conclusion that NOCIS is a promising method for calculating core excitations though it lacks dynamical correlation.

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TABLE I. Comparisons of K-edge calculation errors for several molecules using CIS, Δ-SCF, Δ-DFT, and NOCIS with experimental values, along with the mean signed error (MSE) and root-mean-squared error (RMSE). Calculations were done in the aug-cc-pCVTZ[3,4] basis and all results are in eV.

Molecule	Experiment	CIS	Δ-SCF	Δ-DFT[a]	Δ-DFT[b]	TDDFT[c]	NOCIS
C2H4 C(1s)	284.7[5]	10.10	10.44	-4.50	2.10	3.26	1.70
C2H2 C(1s)	285.9[5]	10.10	9.97	-1.93	4.62	0.27	1.26
H2CO C(1s)	286[7]	8.24	4.94	-0.70	0.71	-0.48	2.01
C2N2 C(1s)	286.3[17]	10.11	7.07	-5.05	1.50	0.17	1.75
HCN C(1s)	286.37[12]	9.52	2.77	-0.46	0.93	0.11	1.71
C2H6 C(1s)	286.9[5]	12.86	7.48	-4.88	1.70	0.45	0.52
CO C(1s)	287.4[10]	6.93	-0.34	-1.01	0.40	-1.34	1.70
CH3OH C(1s)	287.92[11]	11.69	0.70	0.07	1.59	0.58	1.07
CH4 C(1s)	288.1[6]	11.66	-1.17	-1.60	-0.13	0.03	-0.83
CO2 C(1s)	290.8[8]	7.53	3.90	1.48	3.46	-1.06	2.12
C2N2 N(1s)	398.9[17]	12.77	10.74	-5.45	2.26	0.38	1.13
HCN N(1s)	399.7[12]	12.26	2.59	-0.71	0.64	0.21	1.04
NH3 N(1s)	400.8[13]	15.29	-0.13	-0.60	0.84	0.72	0.30
N2 N(1s)	400.96[14]	11.11	16.45	-1.07	1.77	-0.45	1.16
N2O Nt(1s)	401.1[9]	12.22	3.09	-1.11	0.19	0.10	1.09
N2O Nc(1s)	404.8[9]	10.90	5.12	-1.52	-0.19	-0.70	1.14
H2CO O(1s)	530.8[7]	15.12	3.65	-0.75	0.35	0.07	0.70
H2O O(1s)	534[13]	17.10	-0.38	-0.76	0.52	0.48	0.15
CH3OH O(1s)	534.07[11]	17.20	-0.40	-0.62	0.64	0.73	0.22
CO O(1s)	534.2[10]	15.76	-1.44	-1.18	-0.14	0.10	0.11
N2O O(1s)	535[15]	16.43	1.20	-1.30	-0.30	0.58	-0.05
CO2 O(1s)	535.3[15]	16.88	12.28	-0.29	1.04	0.54	0.80
HF F(1s)	682.2[16]	23.30	4.20	4.16	5.20	4.40	4.87
F2 F(1s)	686.5[16]	10.66	7.17	-5.32	-2.72	-5.45	-2.90
MSE		**12.74**	**4.58**	**-1.46**	**1.12**	**0.04**	**0.95**
RMSE		**13.26**	**6.55**	**2.62**	**1.97**	**1.53**	**1.63**

[a] B3LYP

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