Supporting Information for **"Modified Regional Self-Interaction Correction Method Based on Pseudo-Spectral Method"** by A. Nakata, T. Tsuneda, and K. Hirao.

Table S1. 1*s* core-excitation energies (in eV) of C_2H_4, CO_2, N_2, NH_3, H_2O, F_2, and HF molecules and Ne atom calculated by TDDFT with LC-PSRSIC for various *a* values. Cc-pVTZ plus Rydberg basis functions were used. Errors with respect to the experimental data are shown in parentheses.

Molecule	Assignment	LC-PSRSIC with various values of *a*								Exptl.
X = C		*a* value								
		0.89	0.90	0.91	0.92	0.93	0.94	0.95	0.96	
C_2H_4	C1s → π^*	—	288.4	287.4	286.1	284.5	—	279.3	275.1	284.7 [a]
			(+3.7)	(+2.7)	(+1.4)	(-0.2)		(-5.4)	(-9.6)	
	C1s → 3sσ	—	291.5	290.6	289.5	287.9	—	279.6	276.1	287.1 [b]
			(+4.4)	(+3.5)	(+2.4)	(+0.8)		(-7.5)	(-11.0)	
CO_2	C1s → π^*	296.1	295.2	294.2	292.9	291.2	289.1	286.1	282.1	291.0 [c]
		(+5.1)	(+4.2)	(+3.2)	(+1.9)	(+0.2)	(-1.9)	(-4.9)	(-8.9)	
	C1s → 3pπ	298.4	297.5	296.5	295.3	293.7	291.6	288.8	284.8	295.3 [c]
		(+3.1)	(+2.2)	(+1.2)	(-0.0)	(-1.6)	(-3.7)	(-6.5)	(-10.5)	
ME[i]		+2.0	+3.6	+2.6	+1.4	-0.2	-1.4	-6.1	-10.0	
X = N		*a* value								
		0.88	0.89	0.90	0.91	0.92	0.93	0.94	0.95	
N_2	N1s → π^*	407.1	406.0	404.9	403.4	401.8	399.7	397.0	393.5	401.0 [d]
		(+6.1)	(+5.0)	(+3.9)	(+2.4)	(+0.8)	(-1.3)	(-4.0)	(-7.5)	
	N1s → 3pπ	411.5	410.4	409.2	407.7	405.9	403.7	401.0	397.4	407.1 [e]
		(+4.4)	(+3.3)	(+2.1)	(+0.6)	(-1.2)	(-3.4)	(-6.1)	(-9.7)	
NH_3	N1s → 3s	403.4	402.4	401.2	399.8	398.1	395.9	393.1	389.5	400.7 [f]
		(+2.7)	(+1.7)	(+0.5)	(-0.9)	(-2.6)	(-4.8)	(-7.6)	(-11.2)	
	N1s → $3p_e$	405.0	403.9	402.7	401.2	399.5	397.4	394.6	391.0	402.3 [f]
		(+2.7)	(+1.6)	(+0.4)	(-1.1)	(-2.8)	(-4.9)	(-7.7)	(-11.3)	
ME[i]		+4.0	+2.9	+1.7	+0.3	-1.5	-3.6	-6.3	-9.9	
X = O		*a* value								
		0.87	0.88	0.89	0.90	0.91	0.92	0.93	0.94	
CO_2	O1s → π^*	541.1	539.8	538.4	536.6	534.6	532.1	529.1	525.5	534.6 [c]
		(+6.5)	(+5.2)	(+3.8)	(+2.0)	(-0.0)	(-2.5)	(-5.5)	(-9.1)	
	O1s → 3pπ	542.8	541.5	540.0	538.3	536.3	533.9	531.0	527.4	538.4 [c]
		(+4.4)	(+3.1)	(+1.6)	(-0.1)	(-2.1)	(-4.5)	(-7.4)	(-11.0)	
H_2O	O1s → 3s	537.1	535.9	534.5	532.9	530.9	528.6	525.8	522.4	534.0 [f]
		(+3.1)	(+1.9)	(+0.5)	(-1.1)	(-3.1)	(-5.4)	(-8.2)	(-11.6)	
	O1s → $3p_{b2}$	540.6	539.2	537.7	535.9	533.8	531.4	528.4	524.8	535.9 [f]
		(+4.7)	(+3.3)	(+1.8)	(+0.0)	(-2.1)	(-4.5)	(-7.5)	(-11.1)	
ME[i]		+4.7	+3.4	+1.9	+0.2	-1.8	-4.2	-7.2	-10.7	
X = F		*a* value								
		0.85	0.86	0.87	0.88	0.89	0.90	0.91	0.92	
F_2	F1s → σ^*	690.8	689.5	688.1	686.5	684.7	682.5	680.0	677.1	682.2 [g]
		(+8.6)	(+7.3)	(+5.9)	(+4.3)	(+2.5)	(+0.3)	(-2.2)	(-5.1)	
	F1s → 3p	698.0	696.6	695.1	693.4	691.6	689.4	687.0	684.1	693.6 [g]
		(+4.4)	(+3.0)	(+1.5)	(-0.2)	(-2.0)	(-4.2)	(-6.6)	(-9.5)	
HF	F1s → σ^*	690.6	689.4	688.0	686.4	684.6	682.5	680.0	677.2	687.4 [g]
		(+3.2)	(+2.0)	(+0.6)	(-1.0)	(-2.8)	(-4.9)	(-7.4)	(-10.2)	
	F1s → 3p	694.2	692.8	691.3	689.5	687.6	685.4	682.9	679.9	690.8 [g]
		(+3.4)	(+2.0)	(+0.5)	(-1.3)	(-3.2)	(-5.4)	(-7.9)	(-10.9)	
ME[i]		+4.9	+3.6	+2.1	+0.5	-1.4	-3.5	-6.0	-8.9	
X = Ne		*a* value								
		0.80	0.81	0.82	0.83	0.84	0.85	0.86	0.87	
Ne	Ne1s → $3p_{tu}$	872.3	871.0	869.6	868.2	866.6	865.0	863.2	861.3	867.1 [h]
		(+5.2)	(+3.9)	(+2.5)	(+1.1)	(-0.5)	(-2.1)	(-3.9)	(-5.8)	

[a] Ref. 51.
[b] Ref. 52.
[c] Ref. 58.
[d] Ref. 52.
[e] Chen, C. T.; Ma, Y.; Sette, F. Phys. Rev. A 1989, 40, 6737.
[f] Ref. 54.
[g] Ref. 55.
[h] Ref. 56.
[i] Mean errors from the experimental data.