Feshbach-Fano approach for calculation of Auger decay rates using equation-of-motion coupled-cluster wave functions: Numerical examples and benchmarks. Supplementary Material

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1. BASIS-SET DEPENDENCE OF PARTIAL AUGER WIDTHS

TABLE S1: Partial and total Auger decay widths (in meV) for $K-LL$ transitions in core-ionized neon atom. Calculations were done with a plane wave or Coulomb wave (with specified effective charges) and various one-electron basis sets.

	u-6-311+G(3df)		u-aug-cc-pVTZ		u-d-aug-cc-pVTZ	
Channel	Z_{eff} = 0	Z_{eff} = 6.2	Z_{eff} = 0	Z_{eff} = 6.2	Z_{eff} = 0	Z_{eff} = 6.2
^{1}D $(2p^{-2})$	154.9	105.5	154.4	105.0	154.4	105.0
^{1}S $(2p^{-2})$	4.4	12.2	4.4	12.3	4.4	12.3
^{3}P $(2s^{-1}2p^{-1})$	116.5	19.2	116.4	19.0	116.3	19.0
^{1}P $(2s^{-1}2p^{-1})$	4.8	41.5	4.6	41.1	4.6	41.1
^{1}S $(2s^{-2})$	19.0	28.0	19.1	27.8	19.1	27.8
Total	299.6	206.4	298.9	205.2	298.8	205.2

2. NORMS OF TWO-BODY DYSON FUNCTIONS

TABLE S2: Energies (in eV) and squared norms of two-body Dyson functions for the diagram channels in the Auger decay of K−shell ionized water. Squared norm of the two-body Dyson function is calculated as $\|\Gamma\|^2 = \sum_{pqr} {}^{L}\Gamma^{p}_{qr} \cdot {}^{R}\Gamma^{qr}_{p}$

Channel	Energy / eV	$\|\Gamma\|^2$
$^3\mathrm{B}_1(3a_1^{-1}1b_1^{-1})$	499.07	1.91
$^1\mathrm{A}_1(1b_1^{-2})$	498.09	1.92
$^1\mathrm{B}_1(3a_1^{-1}1b_1^{-1})$	496.61	1.91
$^3\mathrm{A}_2(1b_1^{-1}1b_2^{-1})$	495.07	1.90
$^1\mathrm{A}_1(3a_1^{-2})$	493.49	1.91
$^1\mathrm{A}_2(1b_1^{-1}1b_2^{-1})$	493.31	1.90
$^3\mathrm{B}_2(3a_1^{-1}1b_2^{-1})$	493.17	1.90
$^1\mathrm{B}_2(3a_1^{-1}1b_2^{-1})$	491.04	1.91
$^1\mathrm{A}_1(1b_2^{-2})$	486.32	1.91
$^3\mathrm{B}_1(2a_1^{-1}1b_1^{-1})$	480.47	1.86
$^3\mathrm{A}_1(2a_1^{-1}3a_1^{-1})$	478.69	1.85
$^3\mathrm{B}_2(2a_1^{-1}1b_2^{-1})$	474.79	1.83
$^1\mathrm{B}_1(2a_1^{-1}1b_1^{-1})$	473.73	1.80
$^1\mathrm{A}_1(2a_1^{-1}3a_1^{-1})$	472.42	1.80
$^1\mathrm{B}_2(2a_1^{-1}1b_2^{-1})$	467.51	1.60
$^1\mathrm{A}_1(2a_1^{-2})$	453.93	1.55

3. PSEUDO-PARTIAL WAVE CONVERGENCE IN CO_2

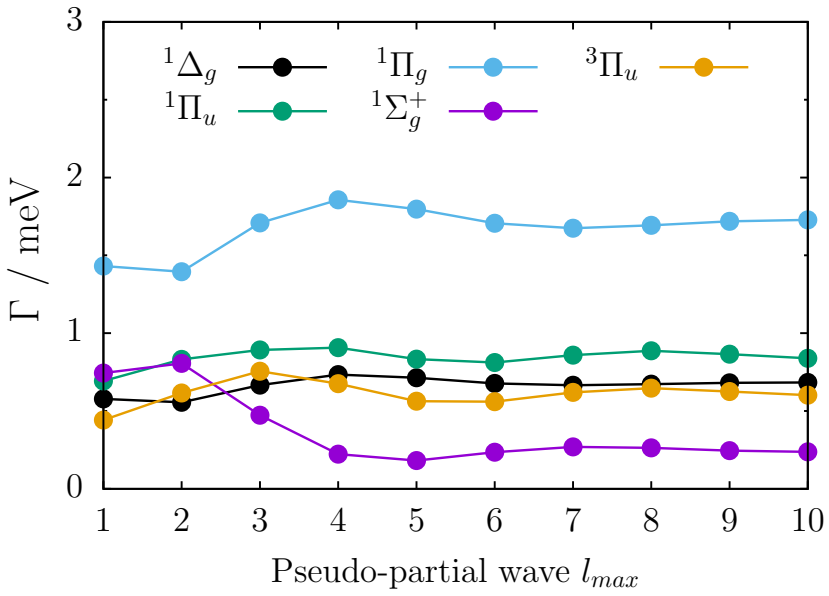

FIG. S1: Convergence of partial Auger decay widths in carbon-edge K–shell ionized CO_2 with respect to pseudo-wave expansion of the Coulomb wave function. Shown intensities correspond to the first 5 channels, listed in Table VI of the main paper. Calculations were done with $Z_{eff} = 3.6$.

4. RELEVANT CARTESIAN GEOMETRIES

Below are molecular geometries employed in the calculations. Given CCSD energies correspond to the ground-state energies of the neutral molecule obtained with fully uncontracted 6-311+G(3df) basis set.

H2O
Nuclear Repulsion Energy = 9.19407001 hartrees
Total CCSD Energy = -76.31560935 hartrees

		Coordinates (Angstroms)		
	Atom	X	Y	Z
1	O	-0.00000	-0.00000	0.11834
2	H	-0.75280	-0.00000	-0.47336
3	H	0.75280	0.00000	-0.47336

CH4
Nuclear Repulsion Energy = 13.48070421 hartrees
Total CCSD Energy = -40.40690653 hartrees

		Coordinates (Angstroms)		
	Atom	X	Y	Z
1	C	-0.00000	0.00000	0.00000
2	H	-0.00000	1.08633	0.00000
3	H	1.02420	-0.36211	-0.00000
4	H	-0.51210	-0.36211	0.88698
5	H	-0.51210	-0.36211	-0.88698

CO2
Nuclear Repulsion Energy = 57.88171895 hartrees
Total CCSD Energy = -188.31330882 hartrees

		Coordinates (Angstroms)		
	Atom	X	Y	Z
1	C	0.00000	0.00000	0.00000
2	O	0.00000	0.00000	1.17022
3	O	0.00000	0.00000	-1.17022