

Supplementary Information

Supplemental data S1 Cell gas indices.

Cell gas	He	H ₂	Ne	Ar	O ₂	N ₂	Kr	Xe
Normalized value of λ	1.00	1.59	1.40	2.77	2.73	2.96	3.60	4.94
α (eV)	24.59 (IP)	4.52 (BE)	21.56 (IP)	15.76 (IP)	5.16 (BE)	9.79 (BE)	14.00 (IP)	12.13 (IP)
H	-46.3	-6.0	-235.9	-251.7	-16.2	-531.9	-127.3	1002.3
He	0.0	37.0	13.2	151.4	1212.4	-21.6	494.9	1252.2
Li	-37.0	-6.8	-219.2	-552.6	-309.1	-470.5	-1250.0	-2104.3
Be	-15.2	-22.5	-85.7	-177.2	-27.9	-600.1	-350.8	-452.8
B	-10.5	-20.9	-60.1	-133.0	-388.5	-497.8	-277.0	-400.3
C	-6.0	-13.1	-32.4	-55.6	-239.9	-281.5	-92.2	-63.0
N	-3.2	-6.5	-15.8	-10.9	44.7	-7.8	12.9	124.7
O	-2.6	0.2	-13.4	-14.2	8.4	5.9	-6.9	58.0
F	-1.3	0.5	-5.2	8.1	48.8	47.2	45.7	151.9
Ne	-0.5	0.5	0.0	24.2	38.6	-6.1	86.0	230.6
Na	-12.9	-4.3	-76.5	-194.4	-19.9	-14.2	-442.0	-749.9
Mg	-8.1	-1.2	-46.8	-107.2	26.9	21.0	-228.7	-347.1
Al	-6.5	-1.0	-38.4	-94.7	-34.4	16.9	-211.5	-348.8
Si	-5.2	-0.3	-29.9	-66.6	-4.6	30.6	-139.5	-204.0
P	-3.6	-0.2	-19.7	-37.0	14.1	-28.6	-67.1	-67.5
S	-3.1	1.2	-17.3	-32.8	39.3	2.5	-60.3	-63.0
Cl	-2.1	0.9	-10.8	-13.8	27.9	-10.5	-13.9	24.2

Ar	-1.3	0.2	-5.8	0.0	-8.5	-18.1	18.9	83.7
K	-10.1	-6.5	-60.3	-157.2	-188.2	-331.6	-362.3	-628.3
Ca	-7.2	-0.7	-42.1	-103.4	-125.8	-256.7	-230.4	-378.0
Sc	-5.9	-1.9	-34.6	-83.4	-70.4	-196.8	-183.7	-295.8
Ti	-5.2	-0.4	-30.5	-72.7	10.7	-161.7	-159.1	-253.0
V	-4.8	0.1	-28.0	-67.0	-16.1	-139.6	-147.0	-234.6
Cr	-4.6	-0.5	-26.6	-63.6	-7.4	-130.3	-139.4	-222.2
Mn	-4.0	-0.5	-23.3	-54.0	-13.8	-117.1	-116.1	-178.6
Fe	-3.7	1.0	-21.5	-48.6	7.3	-101.8	-102.8	-153.3
Co	-3.4	-0.4	-19.9	-45.0	-8.8	-93.2	-95.3	-142.2
Ni	-3.4	-0.3	-19.9	-45.7	-9.6	-97.6	-97.5	-148.0
Cu	-3.1	-0.4	-17.8	-40.6	-12.6	-106.9	-86.4	-130.4
Zn	-2.6	-0.3	-14.9	-30.6	-69.3	-118.7	-60.4	-77.1
Ga	-2.9	3.7	-17.1	-42.2	96.5	59.4	-94.2	-155.2
Ge	-2.3	4.2	-13.2	-30.0	114.3	96.5	-63.4	-94.5
As	-1.8	-0.1	-10.1	-20.1	2.8	-16.2	-38.7	-46.2
Se	-1.5	-0.2	-8.7	-17.4	-2.8	47.3	-33.4	-40.3
Br	-1.2	5.7	-6.5	-10.3	163.8	196.1	-15.5	-4.8
Kr	-0.9	5.1	-4.5	-4.1	149.5	197.6	0.0	25.5
Rb	-5.1		-30.4	-79.6			-183.8	-320.1
Sr	-3.8		-22.3	-55.7			-125.3	-208.8

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ARTICLE

Y	-3.5	-20.6	-50.4	475.5*	-112.0	-183.0
Zr	-3.2	-19.0	-45.7	530.7*	-100.4	-161.1
Nb	-3.0	-17.8	-42.5		-93.1	-148.6
Mo	-2.8	-16.1	-38.0		-82.5	-129.5
Tc	-2.6	-14.9	-34.7		-75.0	-116.4
Ru	-2.4	-14.1	-32.8		-70.5	-109.0
Rh	-2.3	-13.4	-30.9	788.6*	-66.4	-101.9
Pd	-2.1	-11.8	-26.1		-54.3	-78.2
Ag	-2.1	-12.0	-27.7		-59.3	-90.4
Cd	-1.8	-10.1	-21.5		-43.3	-58.3
In	-2.0	-12.1	-30.0	995.9*	-67.4	-111.9
Sn	-1.7	-9.8	-22.8		-49.1	-75.9
Sb	-1.4	-8.0	-17.3		-35.5	-49.9
Te	-1.2	-6.8	-14.4		-29.0	-39.0
I	-1.0	-5.7	-10.7		-19.4	-19.7
Xe	-0.8	-4.4	-6.6		-9.3	0.0
Cs	-3.7	-22.3	-58.9		-136.8	-239.7
Ba	-2.9	-17.0	-43.1		-97.7	-165.5
La	-2.1	-12.6	-31.7		-71.4	-119.4
Ce	-2.0	-11.9	-29.9		-67.4	-113.0
Pr	-2.7	-15.9	-39.9		-90.2	-151.5

Nd	-2.2	-12.9	-32.4	-73.1	-122.5
Pm	-2.2	-12.7	-31.9	-71.8	-120.2
Sm	-2.4	-14.2	-35.5	-79.8	-133.2
Eu	-2.3	-13.6	-33.9	-76.3	-127.2
Gd	-2.2	-12.9	-31.5	-70.2	-115.0
Tb	-2.1	-12.5	-31.0	-69.5	-115.2
Dy	-2.1	-12.3	-30.5	-68.3	-112.7
Ho	-2.0	-12.0	-29.6	-66.0	-108.7
Er	-2.0	-11.8	-28.9	-64.3	-105.6
Tm	-1.9	-11.4	-27.9	-62.0	-101.4
Yb	-1.9	-11.1	-27.0	-60.0	-97.8
Lu	-1.9	-11.3	-28.4	-64.2	-107.9
Hf	-1.7	-9.7	-23.1	-50.5	-80.2
Ta	-1.5	-8.7	-20.1	-43.0	-65.7
W	-1.4	-8.1	-18.4	-38.9	-58.1
Re	-1.4	-7.8	-17.7	-37.6	-56.3
Os	-1.3	-7.2	-15.8	-32.6	-46.6
Ir	-1.2	-6.6	-14.1	-28.4	-38.4
Pt	-1.1	-6.4	-13.7	-27.6	-37.3
Au	-1.1	-6.1	-12.8	-25.5	-33.3
Hg	-1.0	-5.3	-10.1	-18.3	-18.7

JAAS

ARTICLE

Tl	-1.1	-6.6	-16.3	-36.4	-59.7
Pb	-1.0	-5.9	-13.7	-29.5	-45.5
Bi	-0.9	-5.5	-12.8	-27.7	-43.0
Po	-0.8	-4.8	-10.5	-21.7	-31.0
At	-0.7	-4.2	-8.8	-17.4	-22.8
Rn	-0.6	-3.3	-6.0	-10.6	-9.7
Fr	-1.9	-11.5	-30.2	-69.9	-121.9
Ra	-1.5	-9.0	-22.7	-51.5	-87.0
Ac	-1.3	-7.9	-20.2	-45.8	-77.6
Th	-1.1	-6.7	-16.2	-36.0	-58.6
Pa	-1.2	-6.9	-17.0	-38.1	-63.1
U	-1.1	-6.4	-15.6	-34.6	-56.7
Np	-1.1	-6.4	-15.5	-34.5	-56.2
Pu	-1.1	-6.4	-15.8	-35.2	-58.0
Am	-1.1	-6.3	-15.6	-34.9	-57.5
Cm	-1.0	-6.2	-15.2	-34.0	-56.1

IP: 1st ionization potential (eV), BE: Bond energy (eV)

* Ref 8: Another calculation model, which is less precise than the DFT, was used.