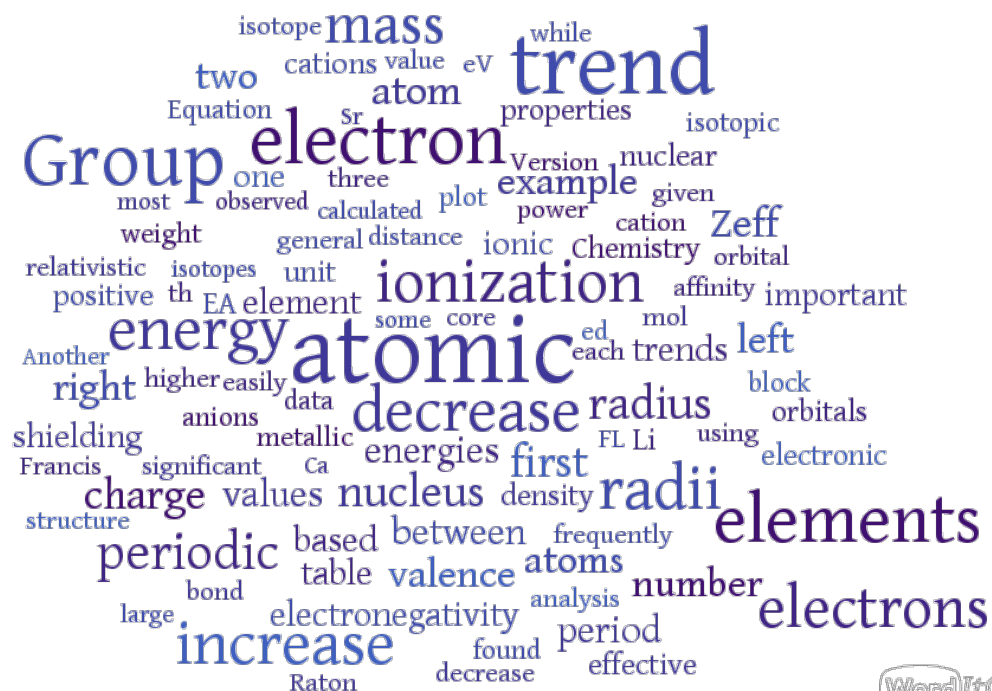


Periodic Trends In Atomic Properties

Trends in fundamental physical properties of atoms/elements



Metals, metalloids and non-metals

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6	58 Ce 140,12	59 Pr 140,907	60 Nd 144,24	61 Pm (147)	62 Sm 150,35	63 Eu 151,96	64 Gd 157,25	65 Tb 158,924	66 Dy 162,5	67 Ho 164,93	68 Er 167,26	69 Tm 168,934	70 Yb 173,04	71 Lu 174,97
7	90 Th 232,038	91 Pa (231)	92 U 238,03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (249)	99 Es (254)	100 Fm (253)	101 Md (256)	102 No (254)	103 Lr (257)

Atomic properties 1: Trends in Z_{eff}

Increasing Z_{eff}

Based on Slater rules!

Increasing Z_{eff}

Constant Slater Z_{eff}

1	1						18
1	H						He
	1.00						1.70
2							
3	Li	Be					Ne
	1.30	1.95					5.85
4							
5	Na	Mg					Ar
	2.20	2.85					6.75
6							
7	K	Ca					Kr
	2.20	2.85					8.25
8							
9	Rb	Sr					Xe
	2.20	2.85					8.25
10							
11	Cs	Ba					Rn
	2.20	2.85					8.25

Increasing Z_{eff}

Clementi's calculated values

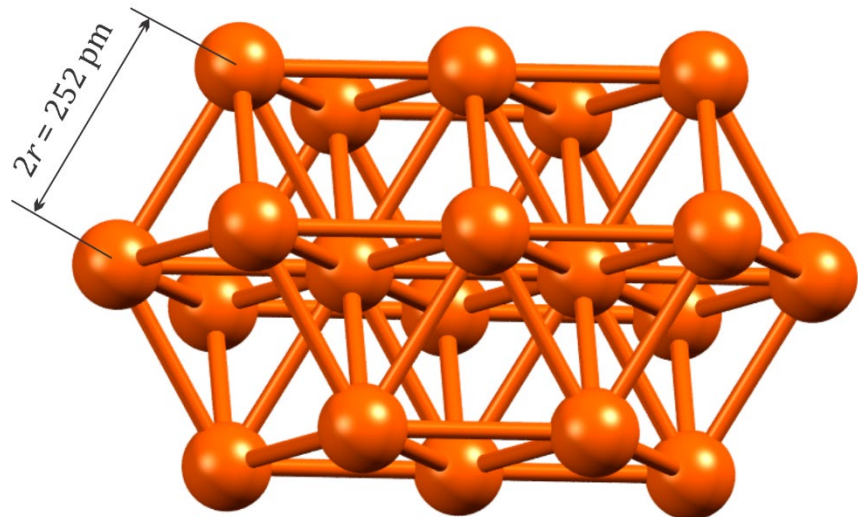
Increasing Z_{eff}

1	1						18
1	H						He
	1.00						1.69
2							
3	Li	Be					Ne
	1.28	1.91					5.76
4							
5	Na	Mg					Ar
	2.51	3.31					6.76
6							
7	K	Ca					Kr
	3.50	4.40					9.77
8							
9	Rb	Sr					Xe
	4.98	6.07					12.41
10							
11	Cs	Ba					Rn
	6.36	7.58					16.08

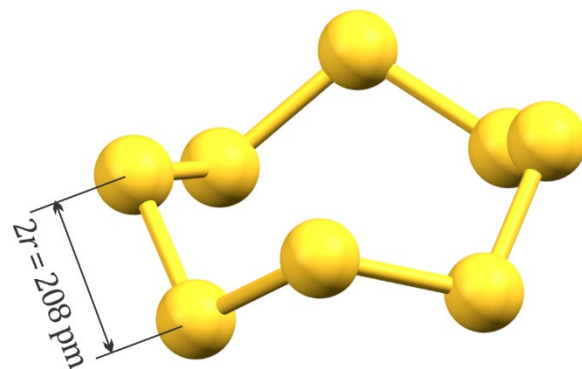
- ➡ **General Trend:** from left to right along the period and down a group, both nuclear and effective nuclear charge *increase*

Atomic Properties 2: Atomic radii

- How do we determine atomic radii? (Definition of atomic radii)



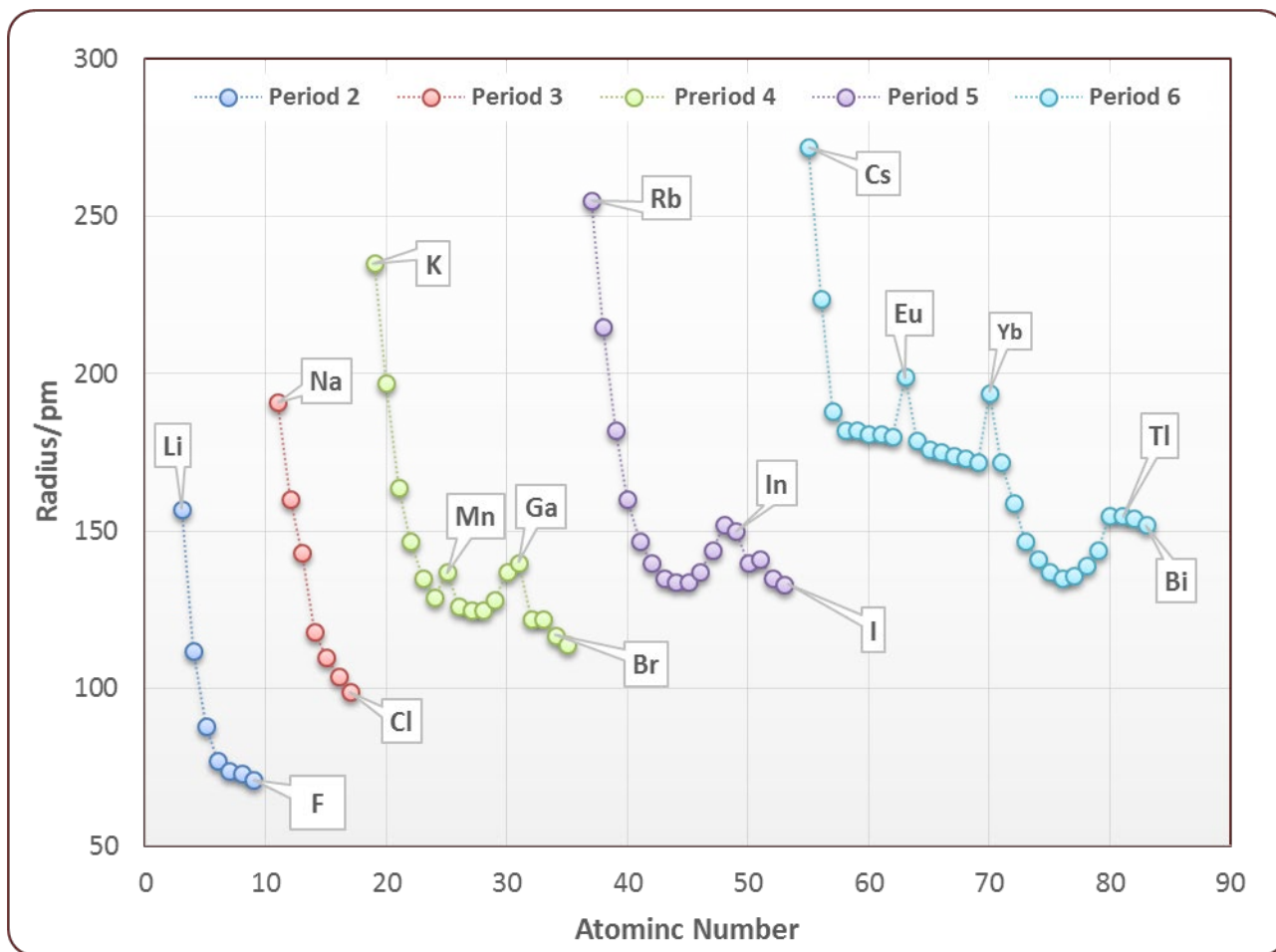
For metallic elements we use *the metallic radius*: half the experimentally determined distance between the centers of nearest neighbor atoms in the solid. Above is the structure of Fe with such a distance indicated.



The *covalent radius* is used for non-metallic elements: half the internuclear distance between the covalently bonded atoms of the same element. Above is the structure of S_8 molecule with such a distance indicated.

Atomic properties 2: Trends in atomic radii

- ➡ **General Trend:** Atomic radii *increase* down a group and *decrease* from left to right along a period!



Atomic Radii: The Lanthanoid Contraction

Atomic radius decreasing

Atomic radius is increasing

All values are in pm

Note the constant radii down the group in d block!

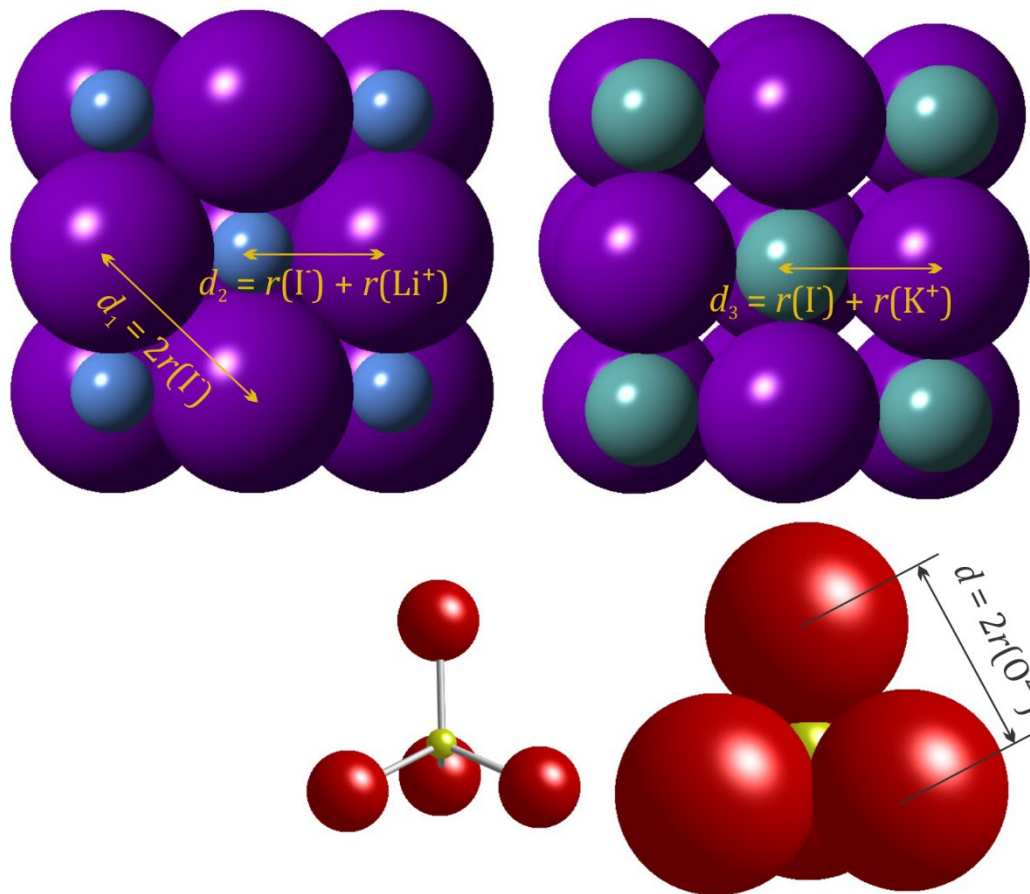
Li	Be												B	C	N	O	F
157	112												88	77	74	73	71
Na	Mg												Al	Si	P	S	Cl
191	160												143	118	110	104	99
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	
235	197	164	147	135	129	137	126	125	125	128	137	140	122	122	117	114	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	
250	215	182	160	147	140	135	134	134	137	144	152	140	140	141	135	133	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi			
272	224	188	159	147	141	137	135	136	139	144	155	155	154	152			

Recall: Lanthanoid elements are found after La and before Hf!

- The 14 lanthanoids follow the trend: their size decreases from left to right, a trend that continues with Hf and the following elements, Lanthanoids fill weakly shielding f orbitals and Z_{eff} increases in their series!

Atomic properties 3: Ionic radii

- How do we determine ionic radii? (Definition of ionic radii)

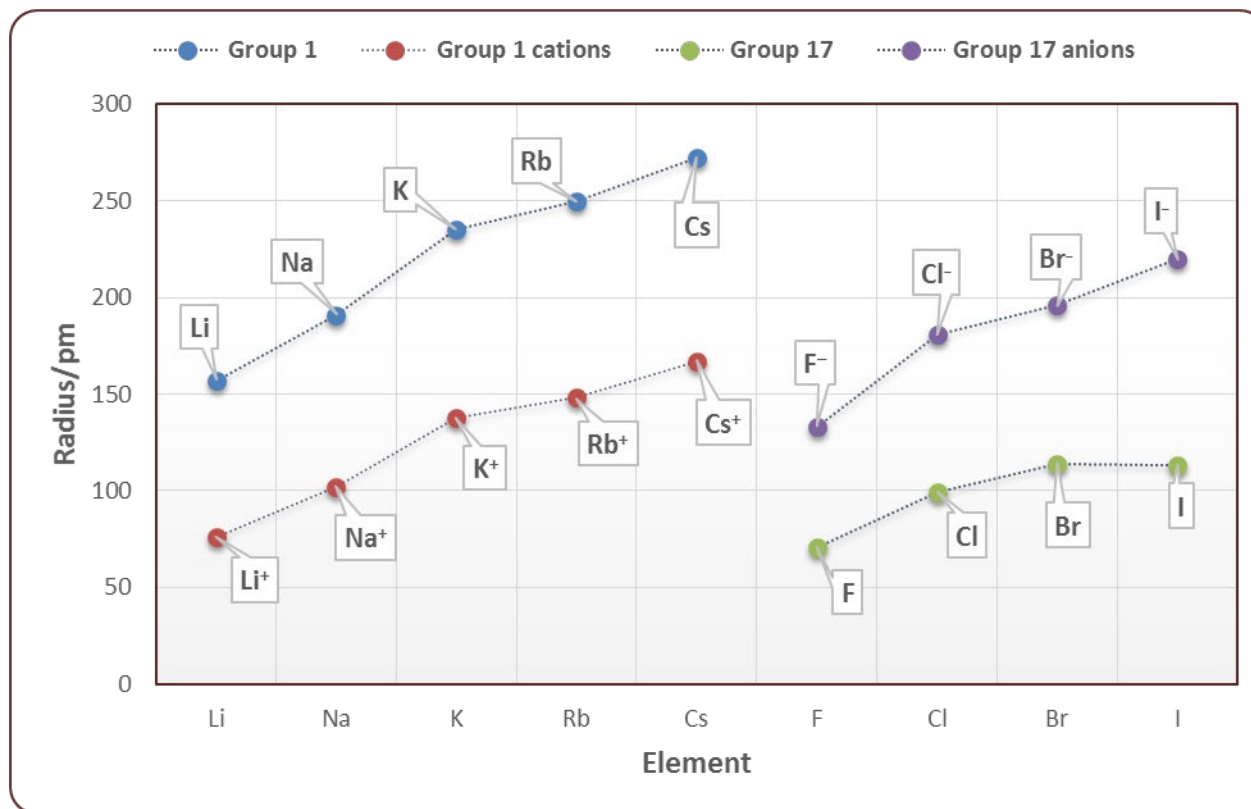


Ionic radii are calculated based on experimentally determined radii for anions. From these, the radii of cations can be determined as $r_+ = r_{\text{total}} - r_-$. For example, Lande's method assumes that anions are in contact when combined with small cations (LiI, as above). Other methods use oxide as a reference (as shown left using SiO₄⁴⁻ as example).

- All tabulated (or plotted) values of both atomic and ionic radii are average values of many measurements and calculations.

Atomic properties 3: Trends in ionic radii

- ➡ **General Trend:** Cations are smaller while anions are larger than their parent, neutral atoms!



- 🔊 **A final note:** Neither atoms or ions have a precise, finite radius.

Atomic Properties 4: Ionization energies

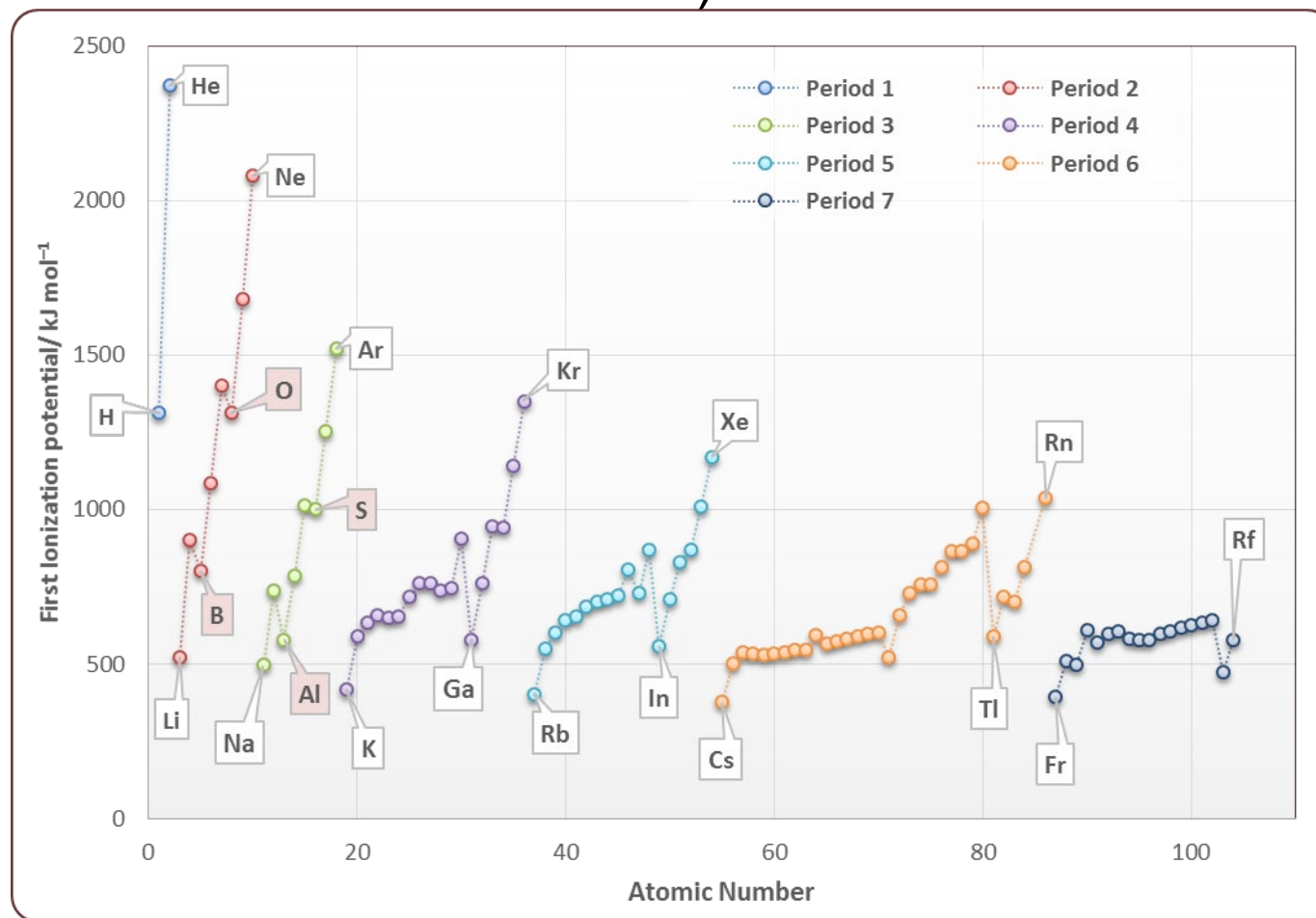
- The energy required to remove one electron from an atom in gas phase is called the *first ionization energy* (potential), I_1 .
- Similarly, the energy required to remove one electron from a singly charged cation (M^+) in gas phase is called the *second ionization energy* (potential), I_2 etc.
- Usually given in electronvolts ($1\text{eV} = 96.485\text{ kJ/mol}$) at $T=0\text{ K}$
- The first ionization energy can be *approximated* from

$$I_1 = \frac{1312.1\text{kJ/mol} \times Z_{\text{eff}}^2}{n^2}$$

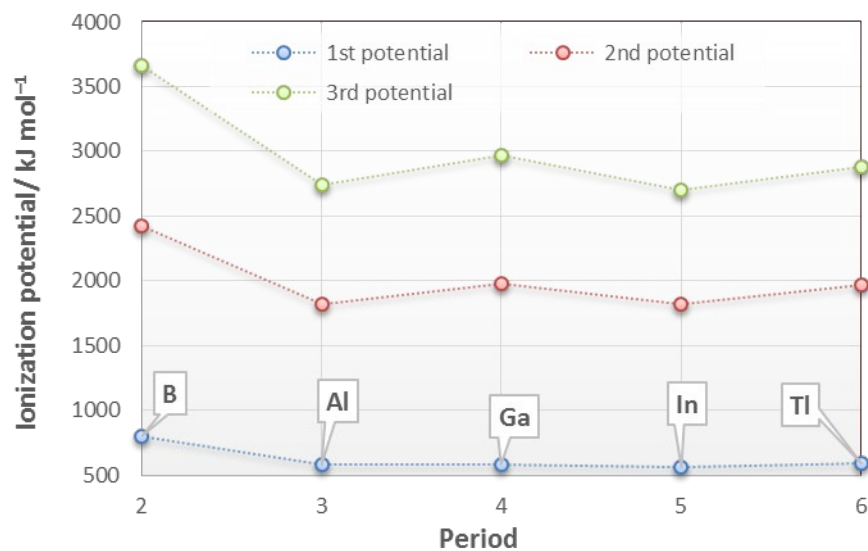
- Note that I_1 depends on *both* Z_{eff} and principal quantum number n
- We can also expect dependence of I on atomic and/or ionic radii: the smaller the radius, the stronger Coulombic attraction.

Atomic Properties 4: Trends in ionization energies (potentials)

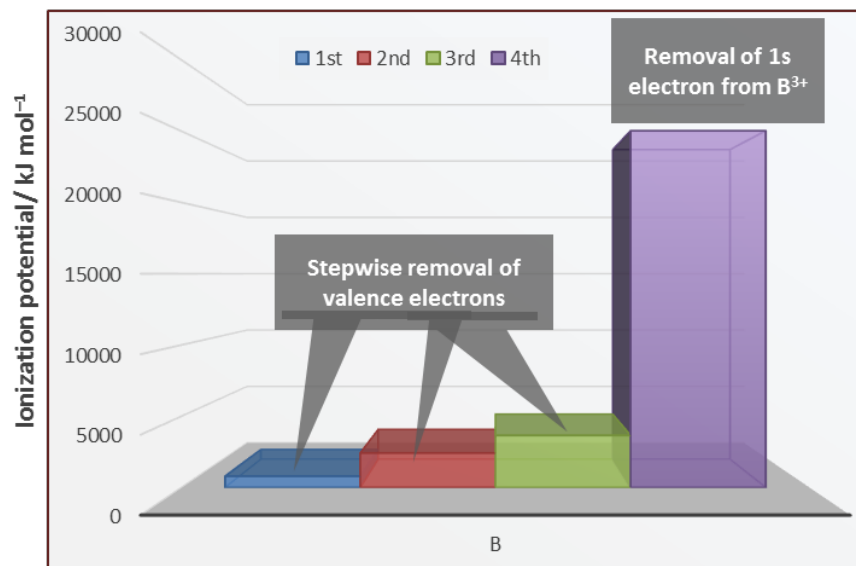
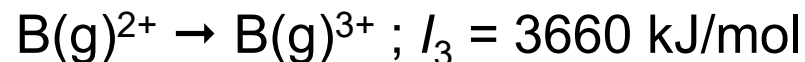
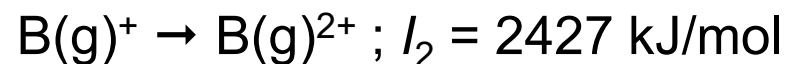
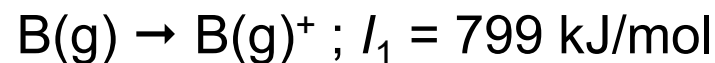
- General Trend: I_1 Increases going from left to right in PTE but decreases going from top to bottom! (note important deviations from the trend marked in red!)



Atomic Properties 4: Trends in ionization energies (potentials) (cont.)



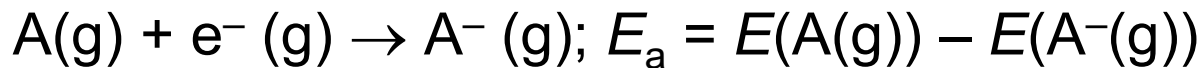
➡ Important trend: successive ionizations of an element require increasingly higher energies, i.e.:



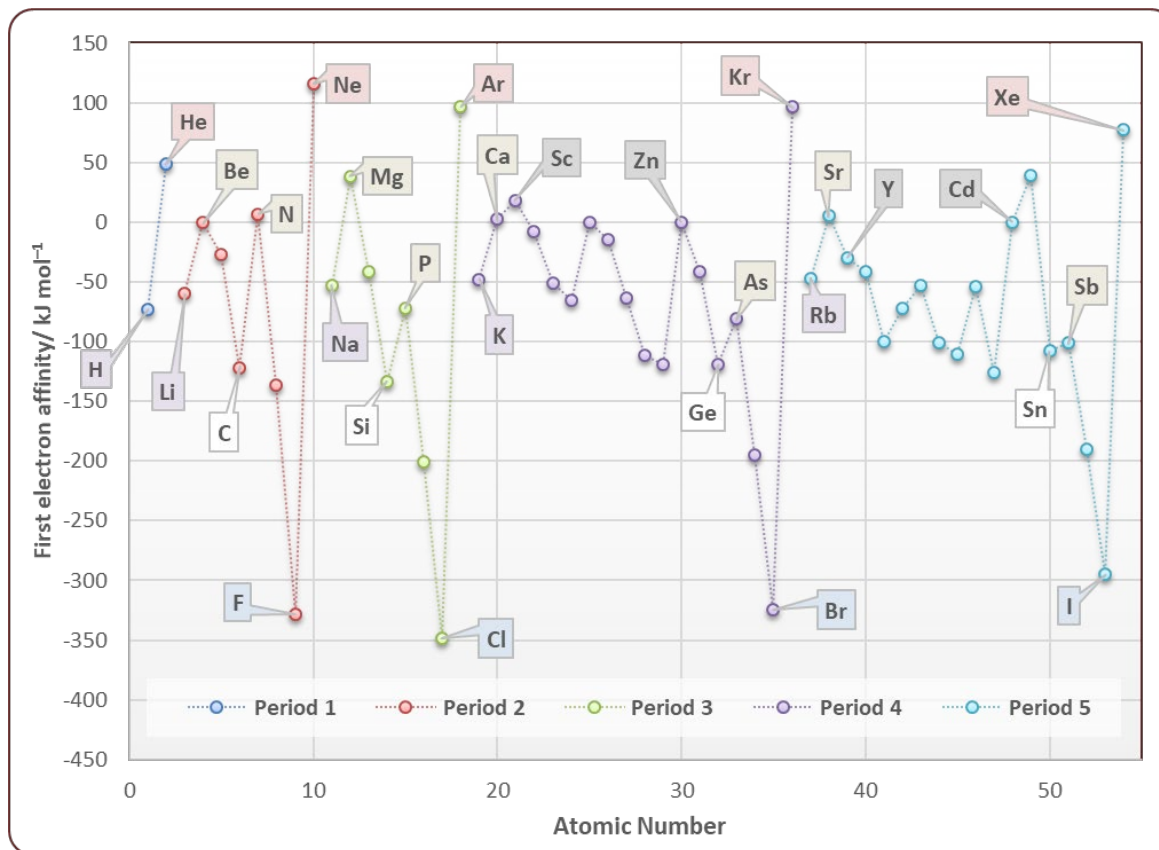
- Once the valence electrons have been removed, the ionization potential undergoes a massive increase

Atomic Properties 5: Electron Affinity

- The *electron affinity* (E_a) is energy change which occurs when an atom in gas phase gains one electron at $T = 0\text{ K}$

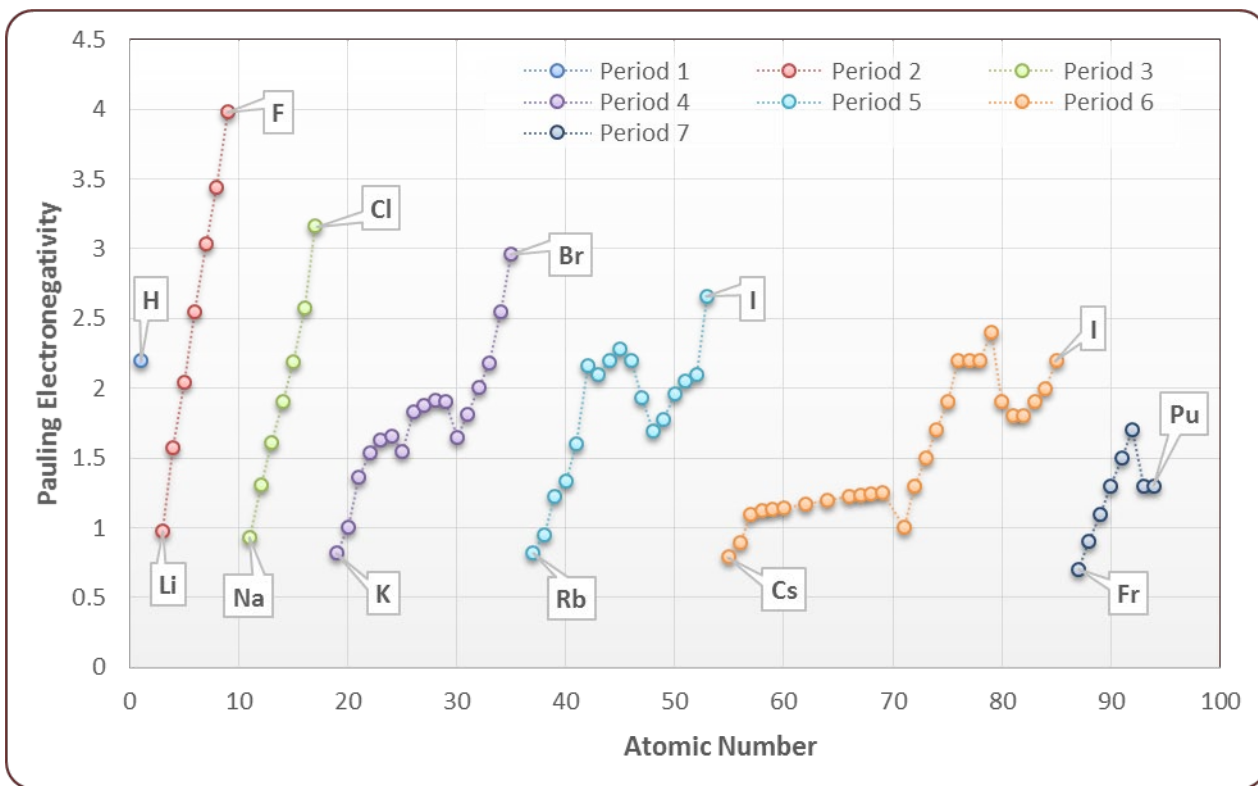


- The trends in E_a are not as clear as with I :



Atomic Properties 6: Electronegativity

- Electronegativity (χ) is the power of an atom of the element to attract electrons to itself when it is a part of a compound
 - Three different definitions of electronegativity: **Pauling**, Miliken and Allerd- Rochow
- ☞ The values differ but the trends are the same for all three: increase from left to right and decrease from top to bottom!



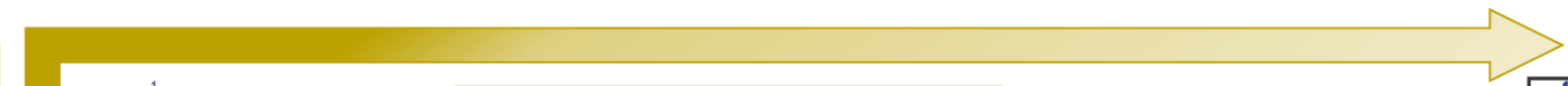

Atomic properties 7: Polarizability

- The **polarizability** (α) of an atom or an ion is its ability to be distorted by an electric field (for example the field of neighboring atom or ion)
- **Fajan's rules:**
 1. Small cations (i.e. Li^+) have polarizing ability (can deform the electronic clouds of other species)
 2. Large anions (I^-) are easily polarized (can be deformed)
 3. Cations that do not have a noble gas configuration (*d*- and *f*- block) are easily polarized
- For example, Li^+ has a higher polarizing ability compared to Cs^+ , while I^- is easier to polarize than F^-

Overview of trends in atomic properties

Top to bottom:

- Increase in: Z_{eff} , EA and ionic radii
- Decrease in: I and χ

Left to right:

- Increase in: Z_{eff} , I , and χ
- Decrease in: atomic radii and EA

1 H 1,00797	2 He 4,0026																										
3 Li 6,989	4 Be 9,0122											5 B 10,811	6 C 12,01115	7 N 14,0067	8 O 15,9994	9 F 18,9984	10 Ne 20,183										
11 Na 22,9898	12 Mg 24,312											13 Al 26,9815	14 Si 28,086	15 P 30,9738	16 S 32,064	17 Cl 35,453	18 Ar 39,948										
19 K 39,102	20 Ca 40,08	21 Sc 44,956	22 Ti 47,90	23 V 50,942	24 Cr 51,996	25 Mn 54,938	26 Fe 55,847	27 Co 58,9332	28 Ni 58,71	29 Cu 63,546	30 Zn 65,37	31 Ga 69,72	32 Ge 72,59	33 As 74,922	34 Se 78,96	35 Br 79,909	36 Kr 83,8										
37 Rb 85,47	38 Sr 87,62	39 Y 88,905	40 Zr 91,22	41 Nb 92,906	42 Mo 95,94	43 Tc (98)	44 Ru 101,07	45 Rh 102,905	46 Pd 106,4	47 Ag 107,87	48 Cd 112,40	49 In 114,82	50 Sn 118,69	51 Sb 121,75	52 Te 127,60	53 I 126,9044	54 Xe 131,3										
55 Cs 132,905	56 Ba 137,34	57 La 138,91	72 Hf 178,49	73 Ta 180,948	74 W 183,85	75 Re 186,2	76 Os 190,2	77 Ir 192,2	78 Pt 195,09	79 Au 196,967	80 Hg 200,59	81 Tl 204,37	82 Pb 207,19	83 Bi 208,98	84 Po (210)	85 At (210)	86 Rn (222)										
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (260)	105 Db (260)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 Ds (269)	111 Rg (272)	112 Cn (277)	113 Nh (282)	114 Fl (285)	115 Mc (289)	116 Lv (289)	117 Ts (294)	118 Og (294)										
s		d										p															

Readings and problems

✓ **Readings:**

- The same for both 6th and 7th edition of the textbook:
 - Remaining part of Chapter 1 from *Shriver's Inorganic Chemistry*
 - Recommended: chapter available on Quercus

✓ Problems:

- From the 6th edition:
 - Examples and Self-Tests 1.8 – 1.11
 - Exercises: 1.19 – 1.21
- From the 7th edition
 - Examples and Self-Tests: 1.9 – 1.12
 - Exercises: 1.19 – 1.21

