This Class

2.2 Aufbau Principle, Shielding

2.3 Periodic Trends

Next Class

Start Chap 3 Simple Bonding Models

Periodic Table of the Elements

$n = 1 \quad l = 0$

$n = 2 \quad l = 0, 1$

$n = 3 \quad l = 0, 1, 2$

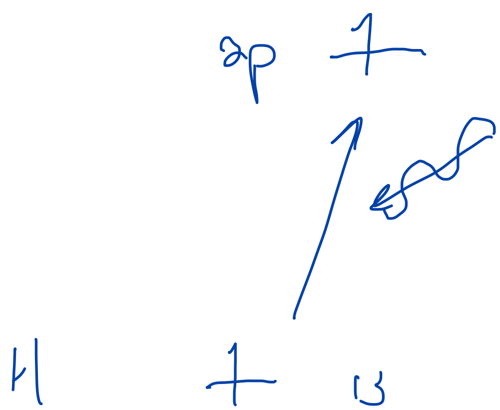
$n = 4 \quad l = 0, 1, 2, 3$

$m_l = 3, 2, 1, 0, -1, -2, -3$

$m_l = 2, 1, 0, -1, -2$

$m_l = 1, 0, -1$

	1	2															3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
①	1 H																															2 He
②	3 Li	4 Be																									5 B	6 C	7 N	8 O	9 F	10 Ne
③	11 Na	12 Mg																									13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
④	19 K	20 Ca															21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
⑤	37 Rb	38 Sr															39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
⑥	55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
⑦	87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og



https://en.wikipedia.org/wiki/Periodic_table spread e^-'s out to lower $e^- - e^-$ repulsion

The Aufbau Principle

1. start in lowest quantum levels
2. Pauli exclusion principle---comes from experiment, not the Schrödinger Equation
3. Hund's Rule of Multiplicity--Multiplicity is the number of unpaired e^-'s + 1

Factors determining the energy of the electron

B $1s^2 2s^2 2p^1$

Penetration and effective nuclear charge

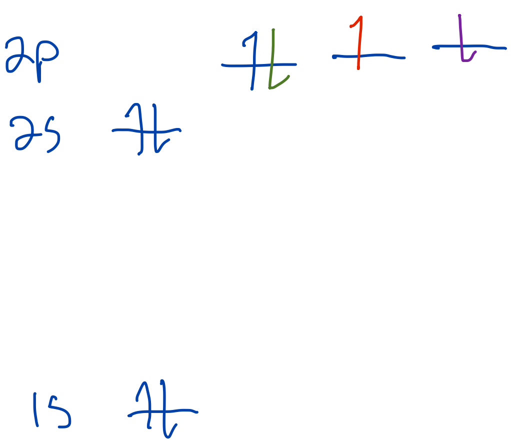
s orbitals penetrate closer to the nucleus. The e^- gets closer to the ⊕ charge

Π_c = coulomb repulsion

-bad

-number of paired electrons

C



if this gap is large it is better to pair

4th e^- pair in lower E s orbital but experience Π_c

when comparing s + p the s is lower in E than the amt. of E $e^- \leftrightarrow e^-$ repulsion causes

The Aufbau Principle
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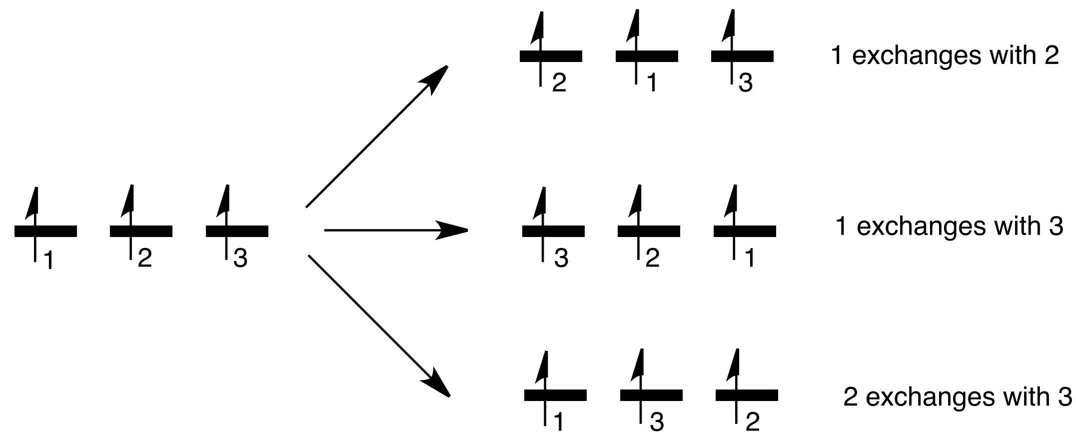
Factors determining the energy of the electron

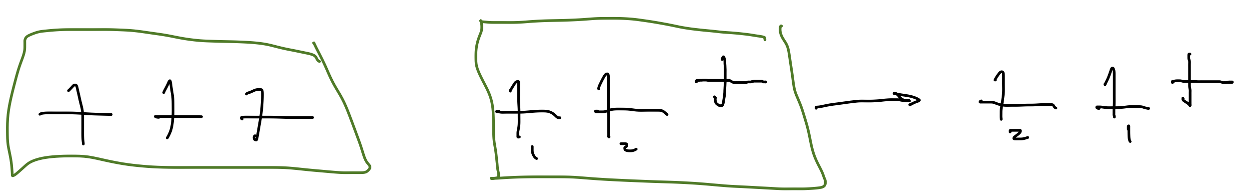
Penetration/effective nuclear charge

Π_c = coulomb repulsion
- bad
-number of paired electrons

Π_e = exchange energy
-good in the case of parallel electrons in an atom
-number of exchanges that can be made and produce identical electron configurations

Exchange energy is **NOT** the exchanges between all possible arrangements (states). Rather, it is the number of possible exhanges of electrons in a single state; thus,





Periodic Table of the Elements

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$Z_{effective}$ is the nuclear charge that outer e^-'s get to experience.

The difference between Z and Z_{eff} is referred to as shielding.

Ga $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^1$

$S = 2 + 8 + 18(.85) + 2(0.35) =$

Slater's Rules for Determining Effective Nuclear Charge

$$Z_{eff} = Z - S$$

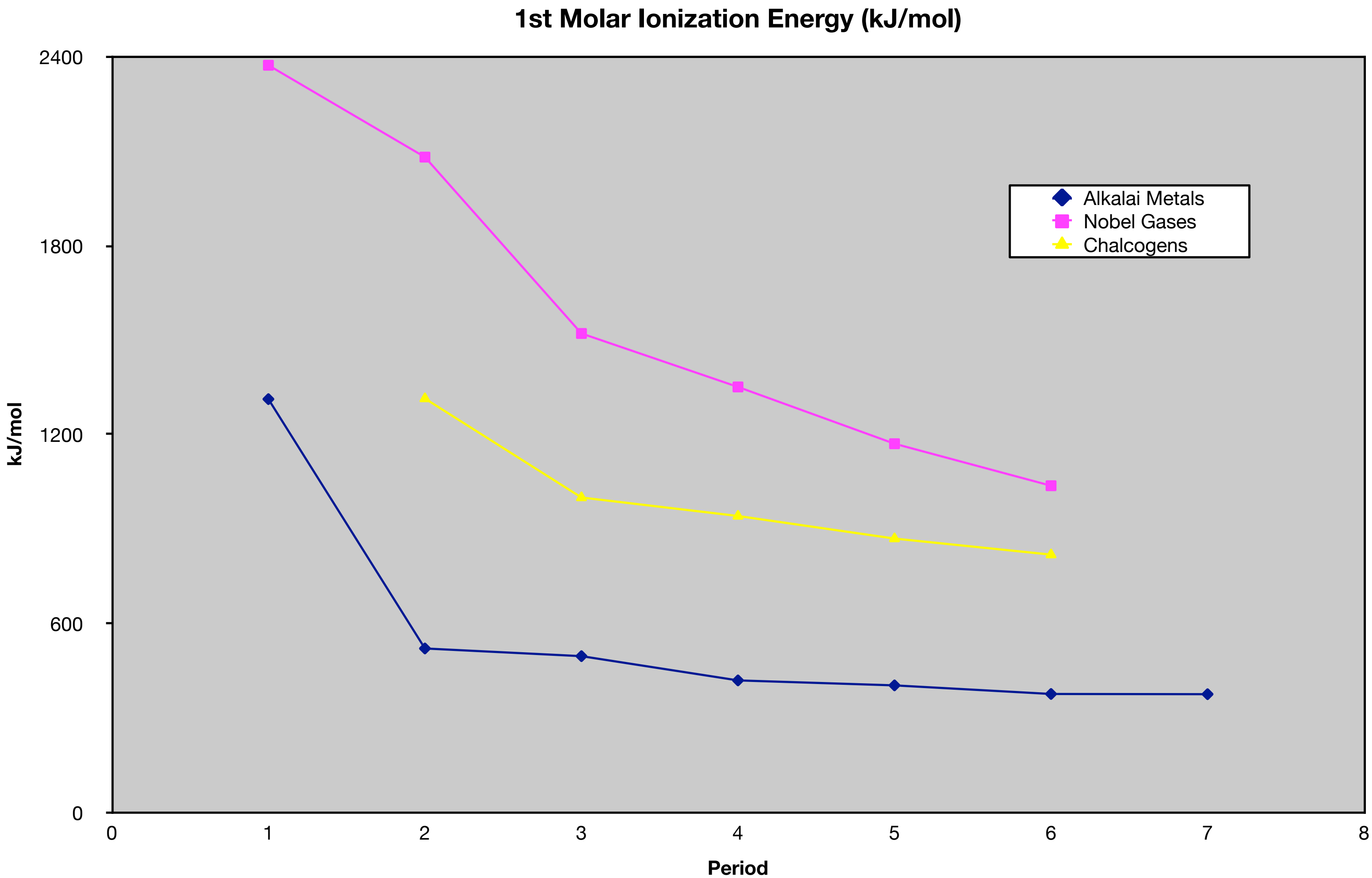
Where Z_{eff} = effective nuclear charge, Z = nuclear charge, and S = shielding constant

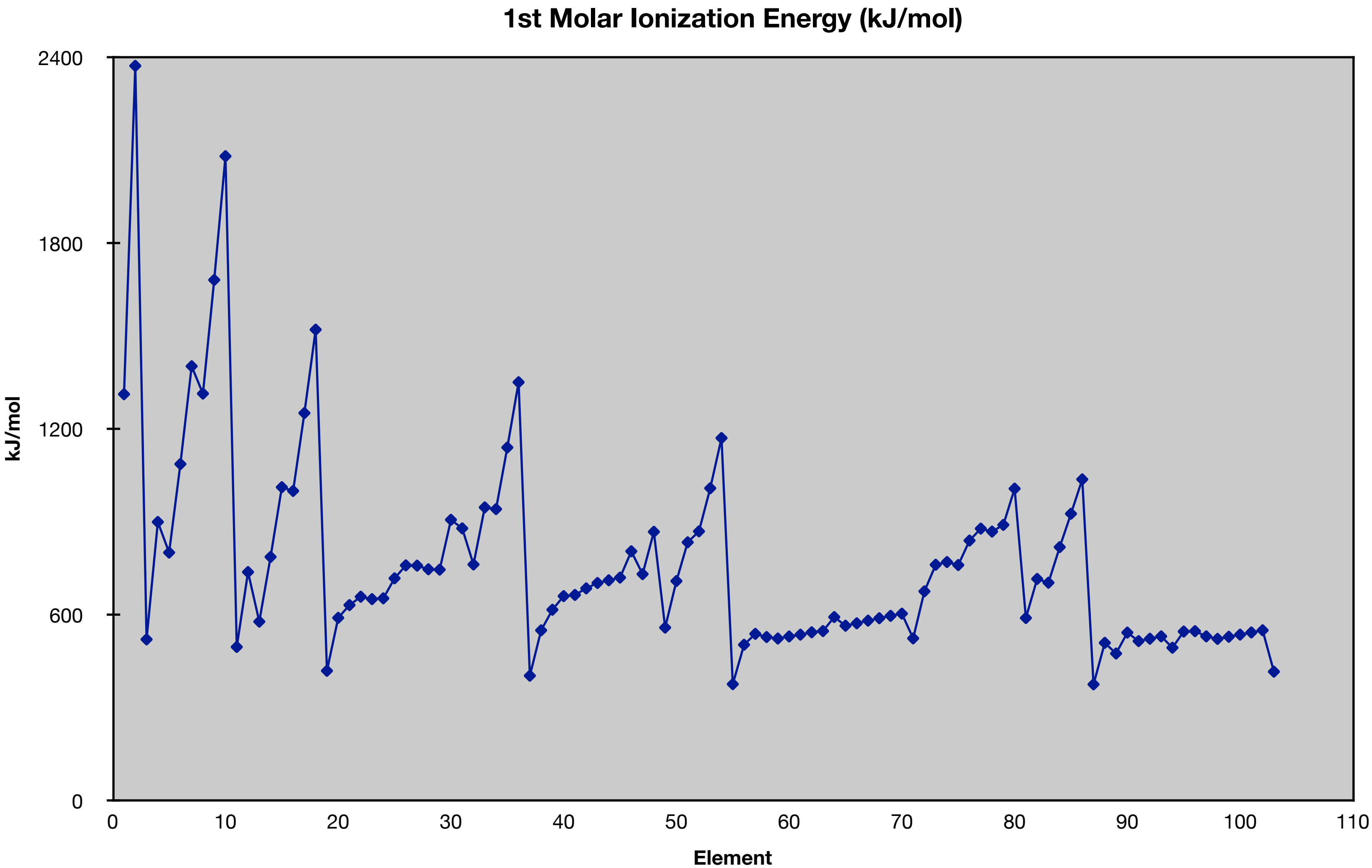
2 e⁻ shield this 3rd e⁻

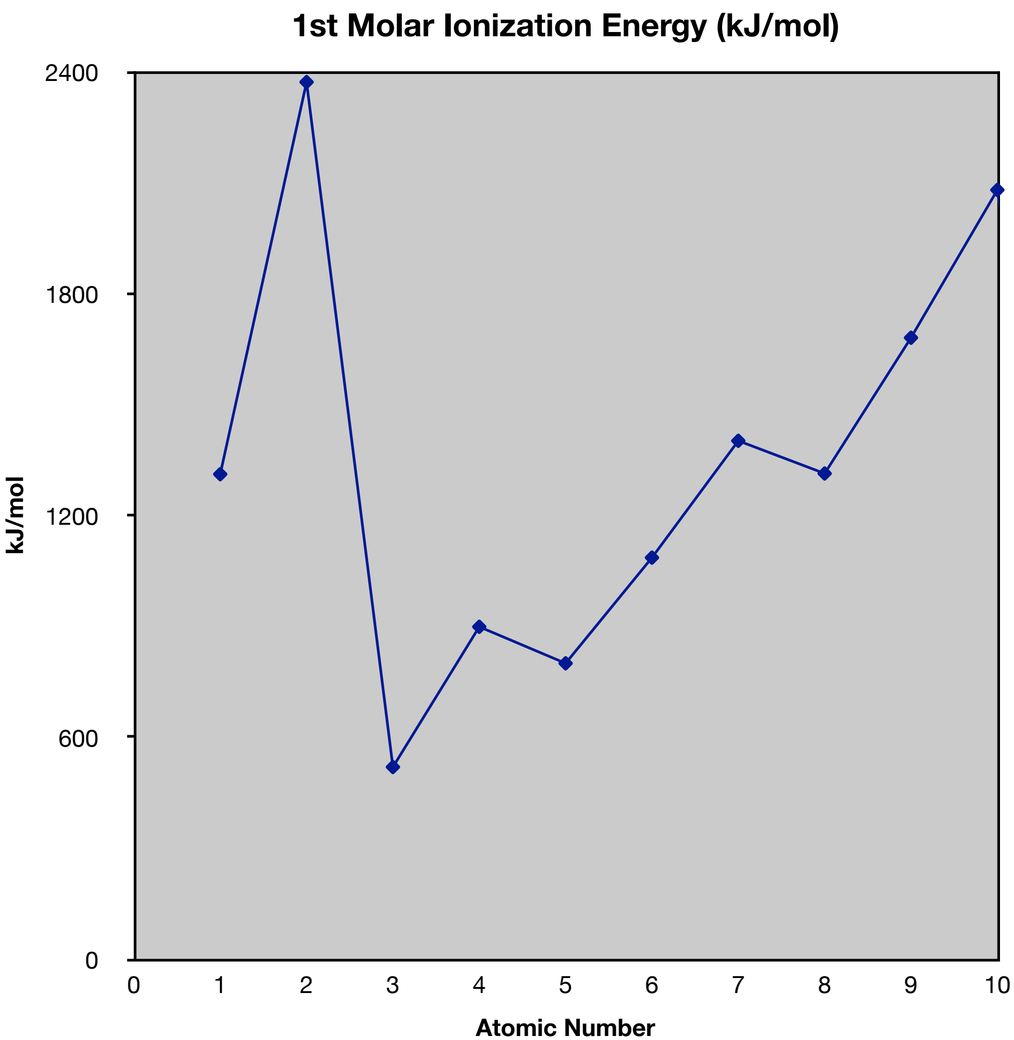
1. group orbitals by n and l   3 e⁻
   (1s) (2s,2p) (3s,3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) (5d) (etc)
2. electrons in groups to the right do not shield electrons to their left
3. S can be determined for *ns* and *np* electrons
   a. each electron in the same group contributes 0.35 to the value of S for other electrons in the same group
      exception, 1s electron contributes 0.30
   b. each electron in n - 1 groups contribute 0.85 to S
   c. each electron in n - 2 groups contribute 1.00 to S
4. for *nd* and *nf*
   a. each electron in the same group contributes 0.35 to the value of S (same as 3a)
   b. each electron in a group to the left contributes 1.00 to S

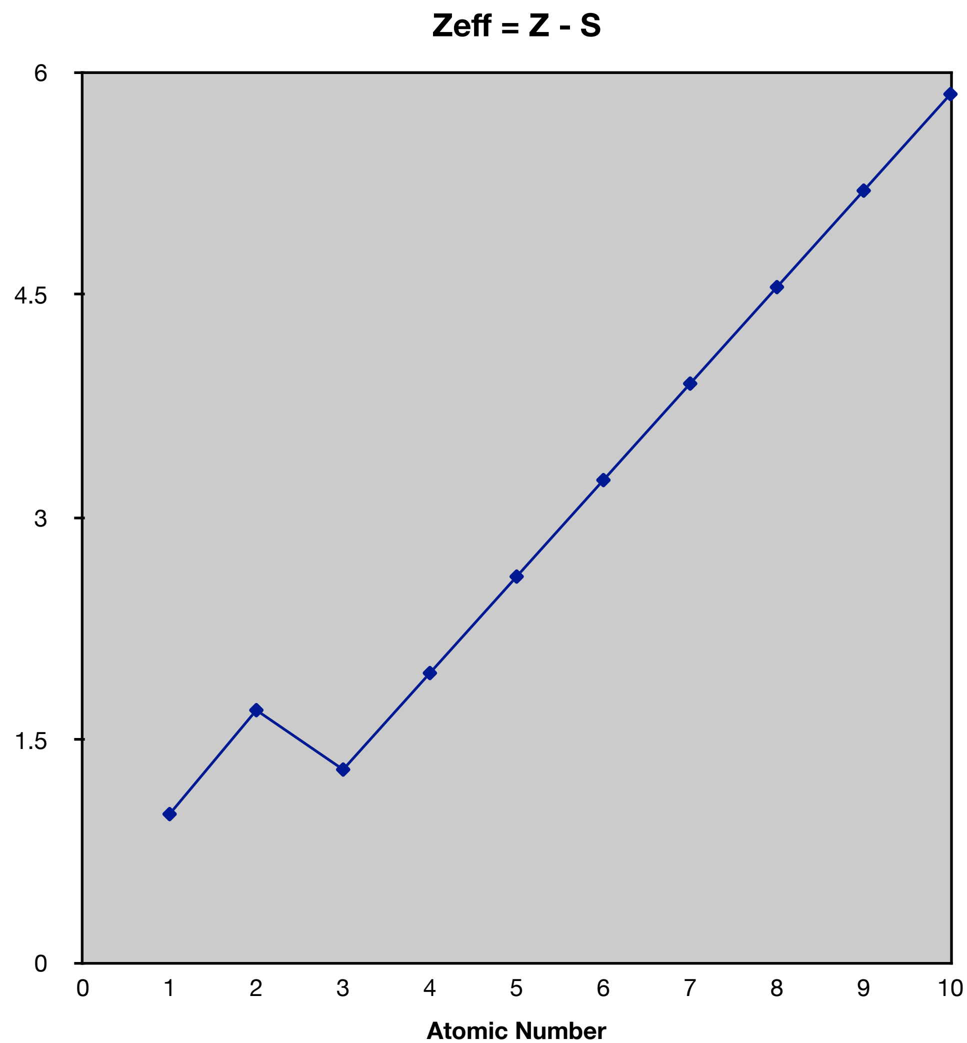
$Z_{effective}$ is the nuclear charge that outer e⁻'s get to experience.

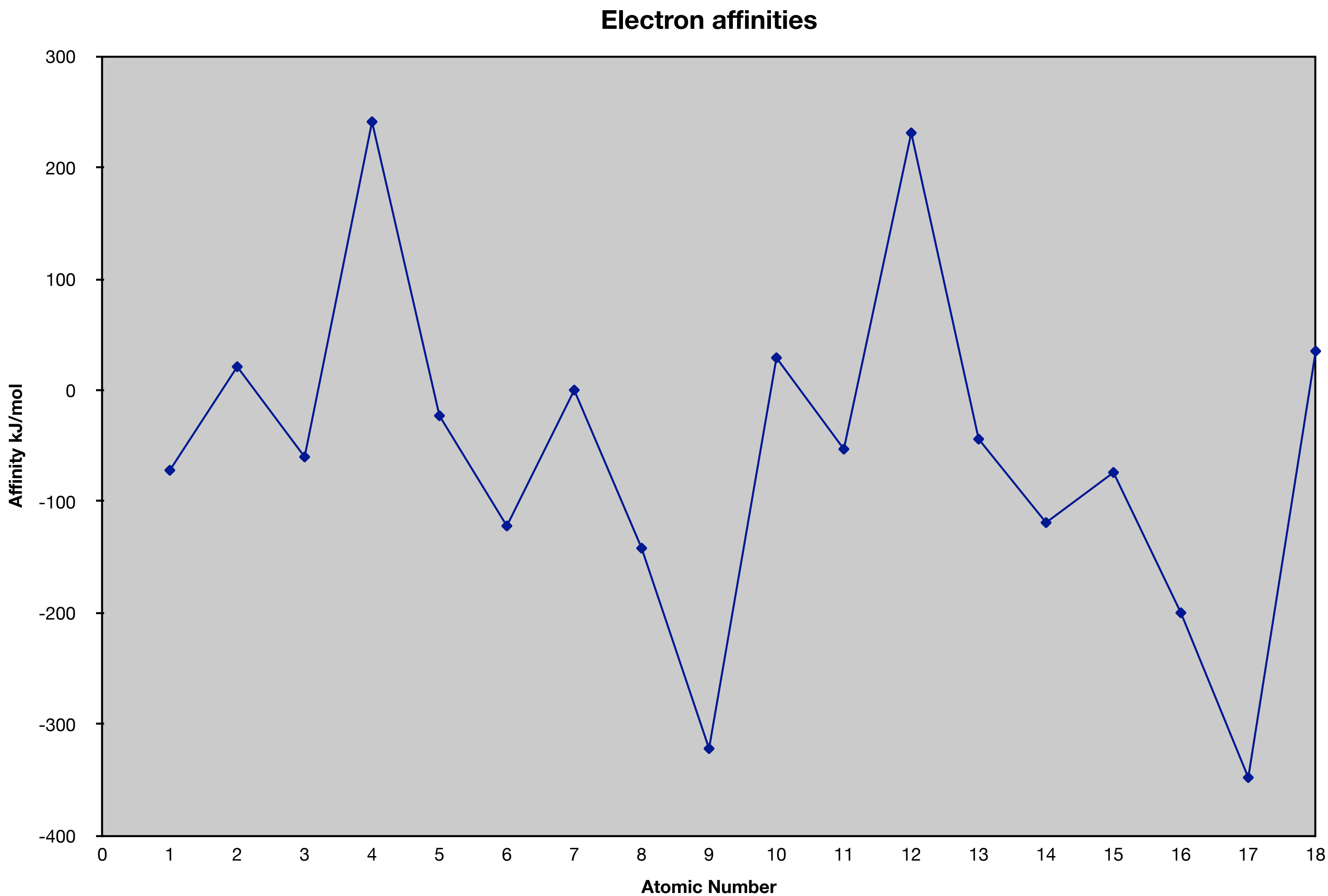
The difference between Z and Z_{eff} is referred to as shielding.


1st Molar Ionization Energy (kJ/mol)
2400
1800
1200
600
0
kJ/mol
0
1
2
3
4
5
6
7
8
Period
Alkalai Metals
Nobel Gases
Chalcogens


1st Molar Ionization Energy (kJ/mol)
kJ/mol
2400
1800
1200
600
0
0
10
20
30
40
50
60
70
80
90
100
110
Element


1st Molar Ionization Energy (kJ/mol)
kJ/mol
2400
1800
1200
600
0
0 1 2 3 4 5 6 7 8 9 10
Atomic Number


Zeff = Z - S
6
4.5
3
1.5
0
0 1 2 3 4 5 6 7 8 9 10
Atomic Number


Electron affinities
300
200
100
0
-100
-200
-300
-400
Affinity kJ/mol
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
Atomic Number