(5) **Today**

2.2.3 The Aufbau Principle

2.2.4 Shielding

Next Class (6)

2.3 Periodic Properties

(7) **Second Class from Today**

2.3 Periodic Properties

3.1 Lewis Structures

3.2 VSEPR

Third Class from Today (8)

3.2 VSEPR

Office Hours Rescheduled to Tuesday

↑ ↑ ↑ vs ↑ ↓ ↑

1. start in lowest quantum levels
2. Pauli exclusion principle
   --- no two electrons in an atom or molecule can have identical quantum numbers
3. Hund's Rule of Multiplicity
   --- multiplicity is the number of unpaired e^-'s + 1
   --- the lowest energy state for electrons in degenerate orbitals is the one with the highest multiplicity
   --- electrons only pair after all degenerate orbitals have been half filled
4. Exchange interaction
   --- spin aligned electrons in degenerate orbitals are lower in energy than those that aren't spin aligned

Rationalizing electron configurations/Factors affecting the energy of the electron

the repulsion experienced by a pair of e^-'s would ↑ the E of the e^-'s

Interactions with nucleus lowers the E of the e^-'s ... the closer the e^- gets the better

Exchange interactions/energy is a favorable interaction

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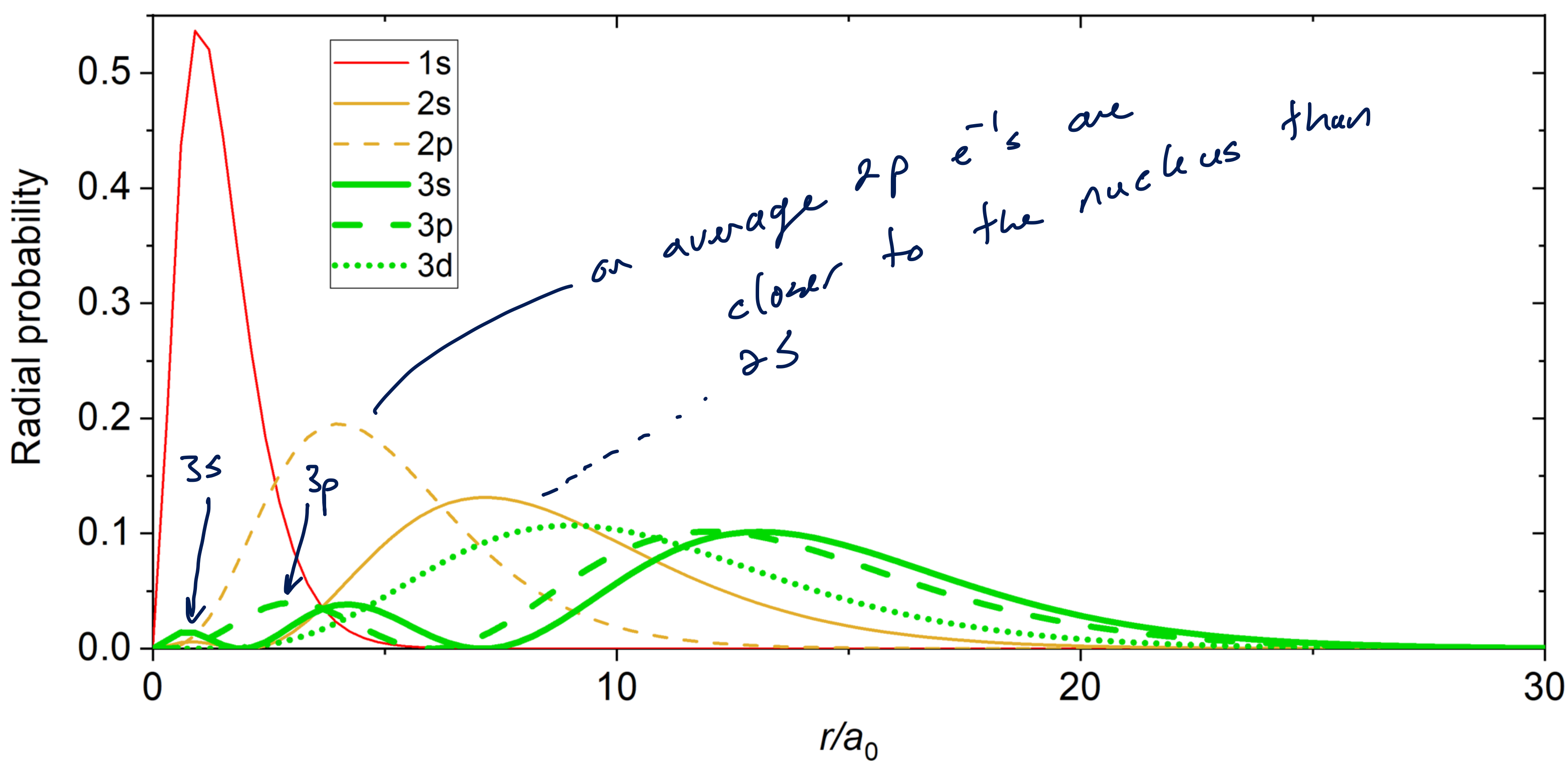
Rationalizing electron configurations/Factors affecting the energy of the electron

Penetration and effective nuclear charge

Π_c = coulomb repulsion
↑
- bad
- number of paired electrons

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

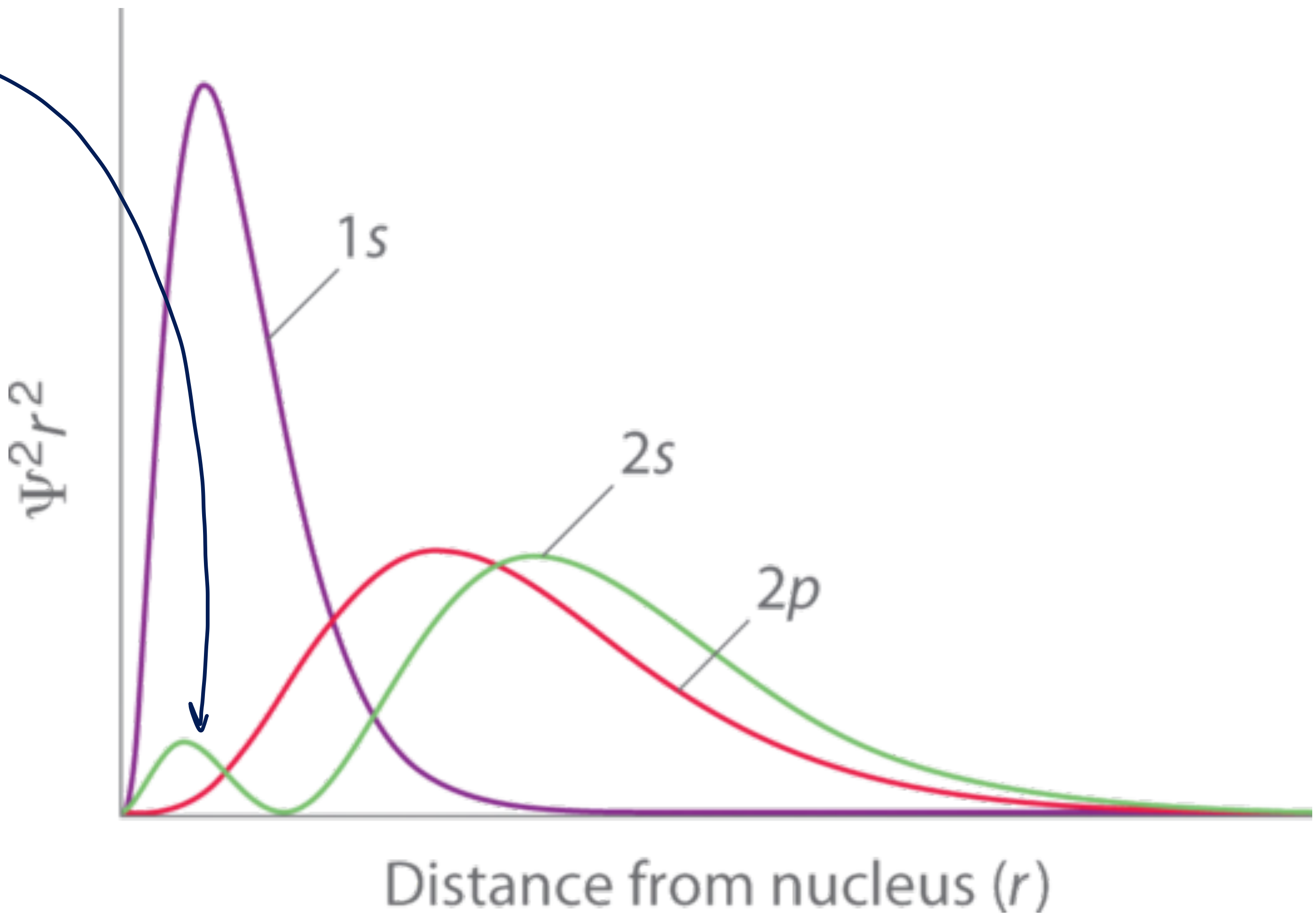
Penetration and effective nuclear charge



Penetration and effective nuclear charge

2s orbitals penentrate farther in to the nucleus than 2p

This penetration makes the 2s lower than the 2p



https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Inorganic_Chemistry_(LibreTexts)/02%3A_Atomic_Structure/2.02%3A_The_Schrodinger_equation_particle_in_a_box_and_atomic_wavefunctions/2.2.04%3A_Shielding accessed 9/15/2023

Periodic Table of the Elements

	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
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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

$n=2 \rightarrow$

Be $1s^2\ 2s^2$

always true for s+p orbitals

2p — — —

2s ⇅

large gap

1s ⇅

I_E smaller than E required to promote e^- so e^-'s are paired

↿ ↿ — —

⇅

promoting this e^- to a 2p orbital would require more E than spin pairing

C $1s^2\ 2s^2 2p^2$

exchange interaction keeps them spin aligned

2p ~~⇅ — —~~ → ↿ ↿ —

2s ⇅

1s ⇅

experience e^- pair repulsion and there is no E gap associated with putting one e^- in a different orbital

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N $1s^2 2s^2 2p^3$

2p ⥮ ↿ — or ↿ ↿ ↿

2s ⥮

1s ⥮

* $e^- - e^-$ is a problem
* fewer exchange interactions

* good... no $e^- - e^-$ pair repulsion
* p orbitals are degenerate (no cost in putting e^- in next available orbital)
* more exchange interactions

4s + 3d are very close in E.

p

s

d

f

3s 3p 3d →

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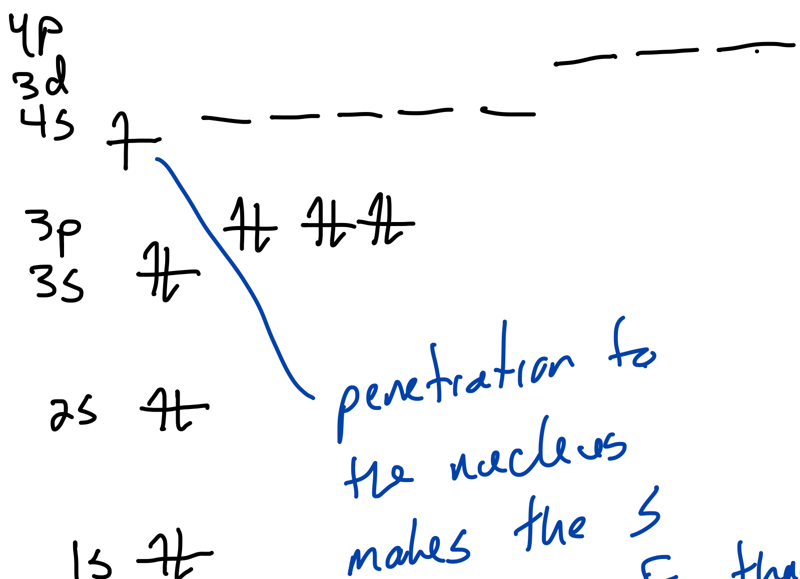
K

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^0$

s orbitals penetrate to the nucleus and start out lower in E than the d orbitals. But as nuclear charge increases s + d get closer together and Π_c + Π_e become more important in determining how orbitals fill



penetration to the nucleus makes the s lower in E than the 3d

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V $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$

$[Ar]\, 4s^2 3d^4$

4p — — —

3d ↑ ↑ ↑ — —

4s ↑↓

no reason to pair e⁻'s in 3d orbitals and experience e⁻-e⁻ repulsion

gap is large enough that Π_c is not a problem in 4s

4p — — —

3d ↑ ↑ ↑ ↑ ↑

4s ↑~~↓~~

e⁻ pair repulsion

4 new exchange interactions

promoting and getting exchange interaction is more favorable than spin pairing in 4s

Slater's Rules for Approximating Effective Nuclear Charge

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

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

1. group orbitals by n and l
   (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

H	He	F

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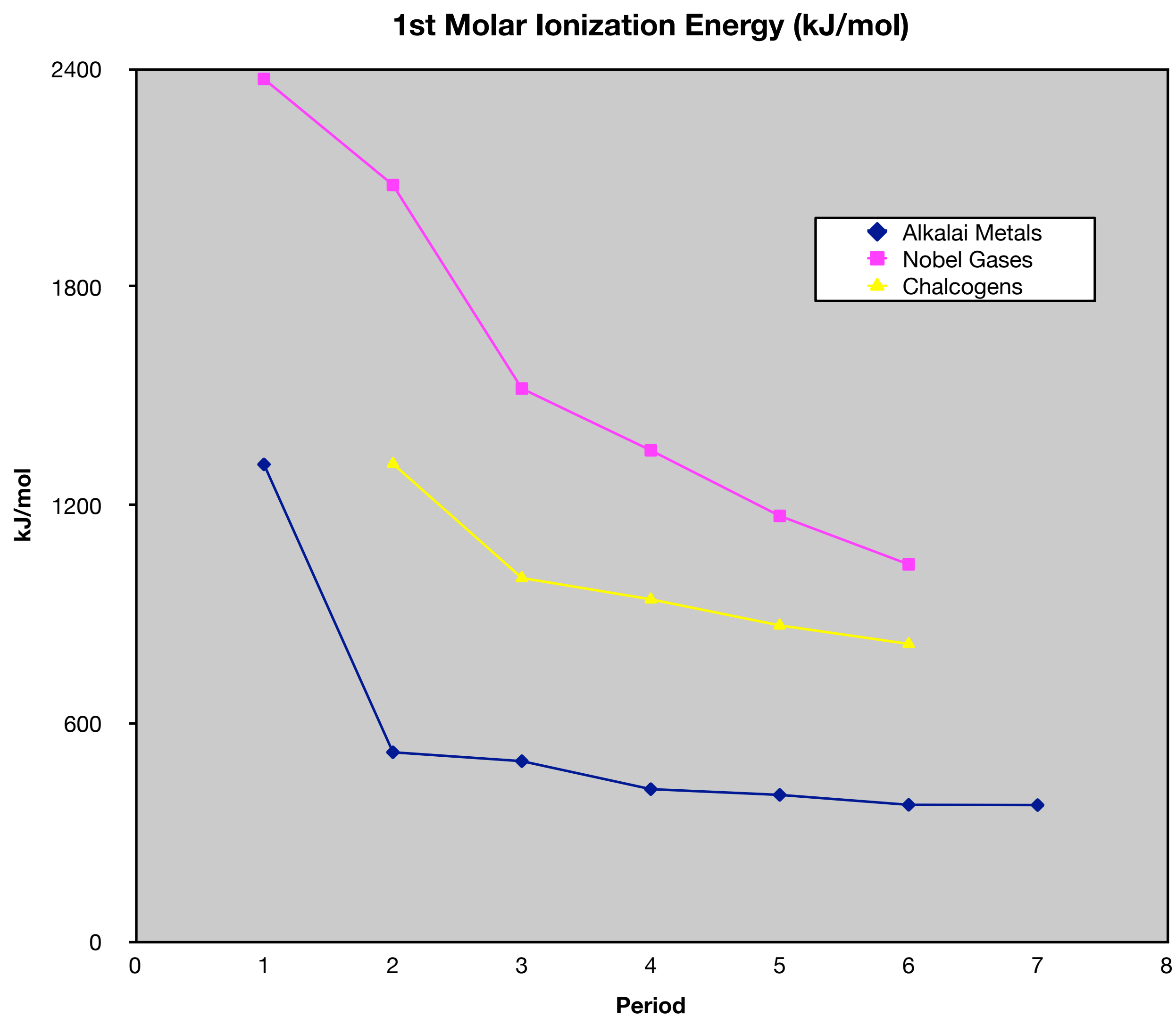
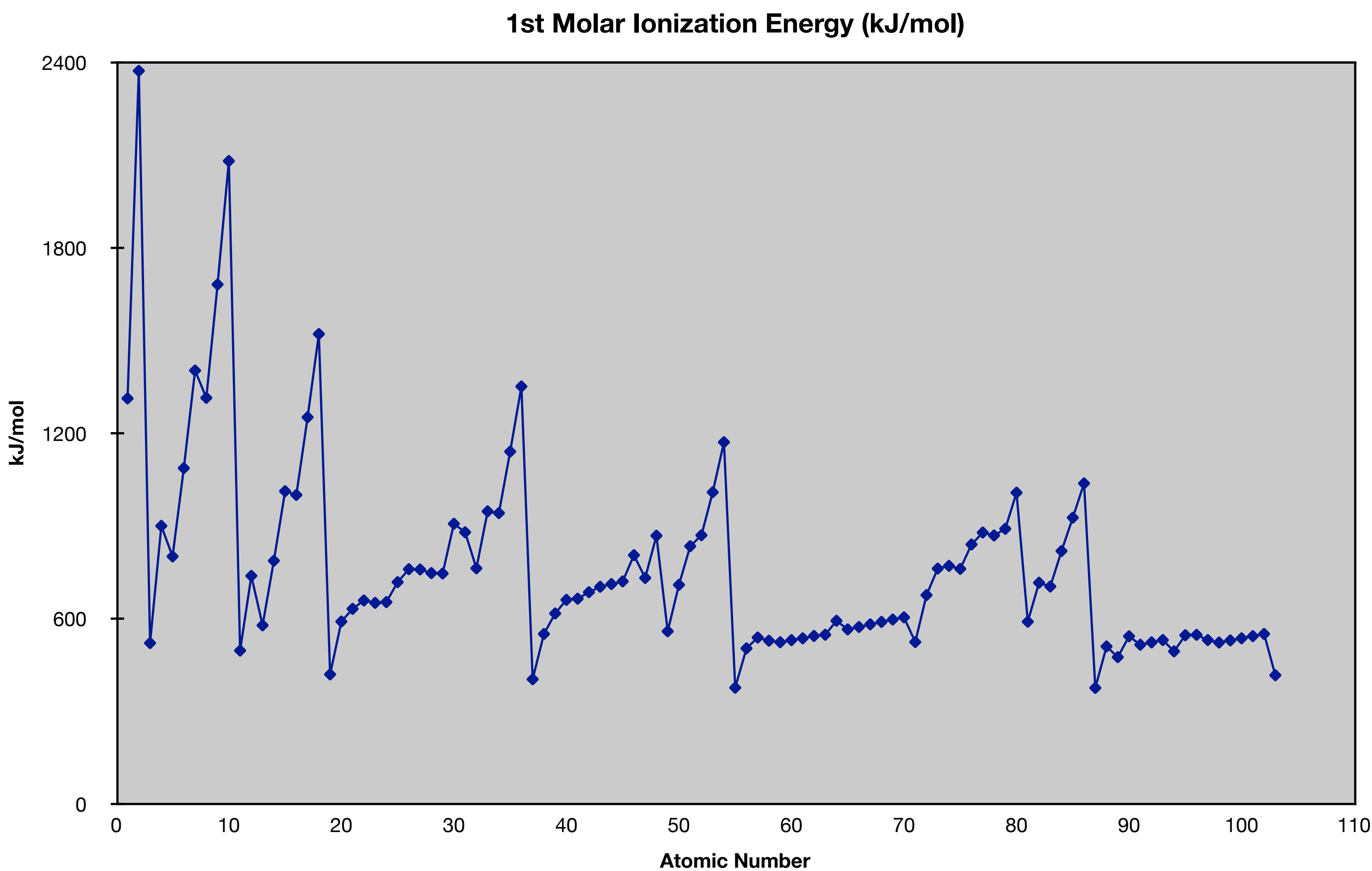
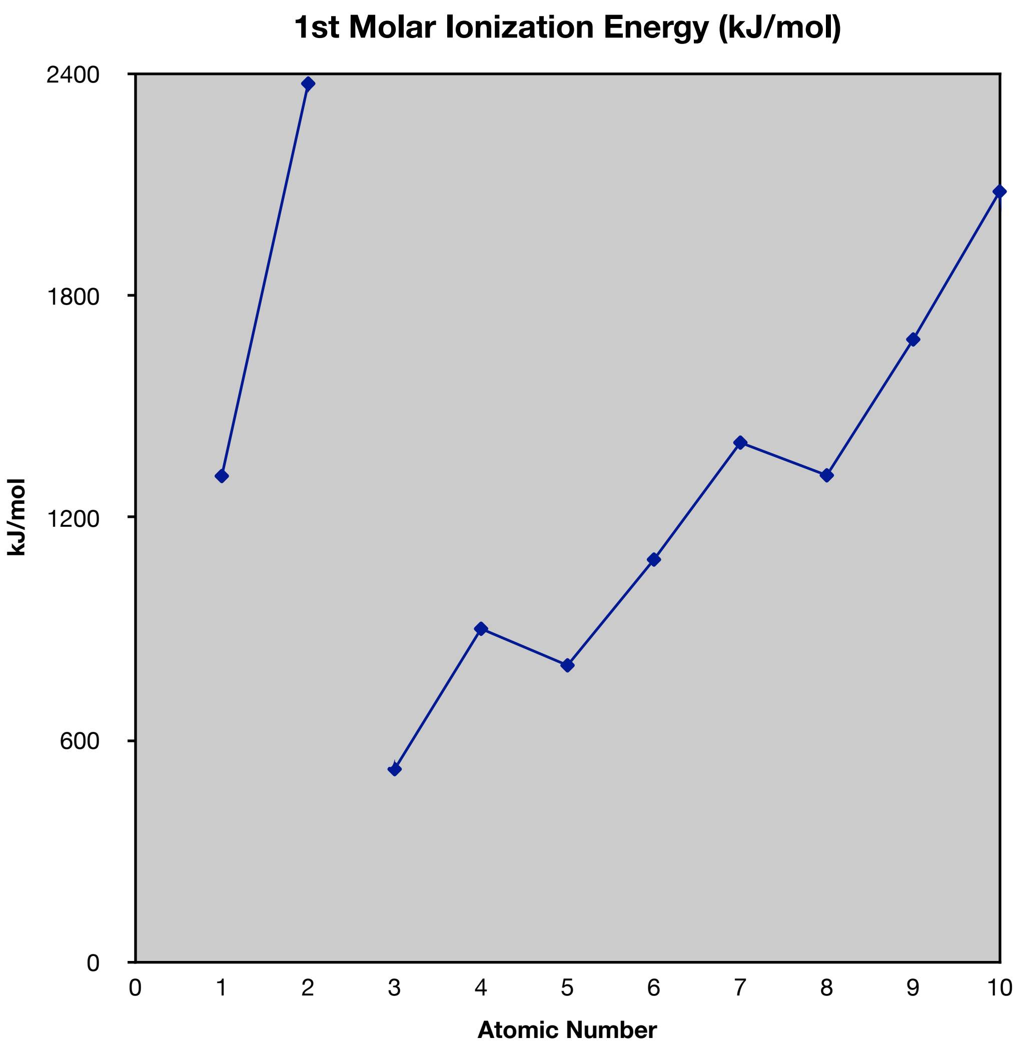
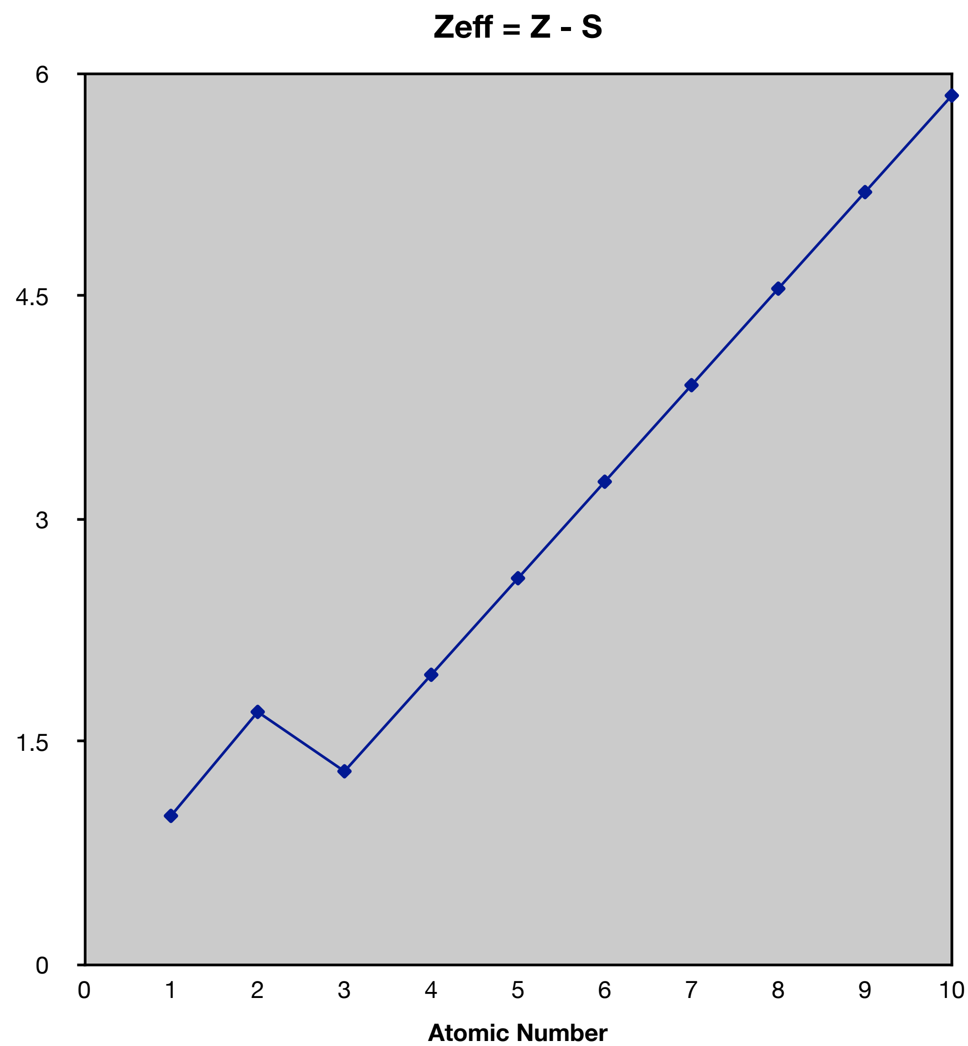
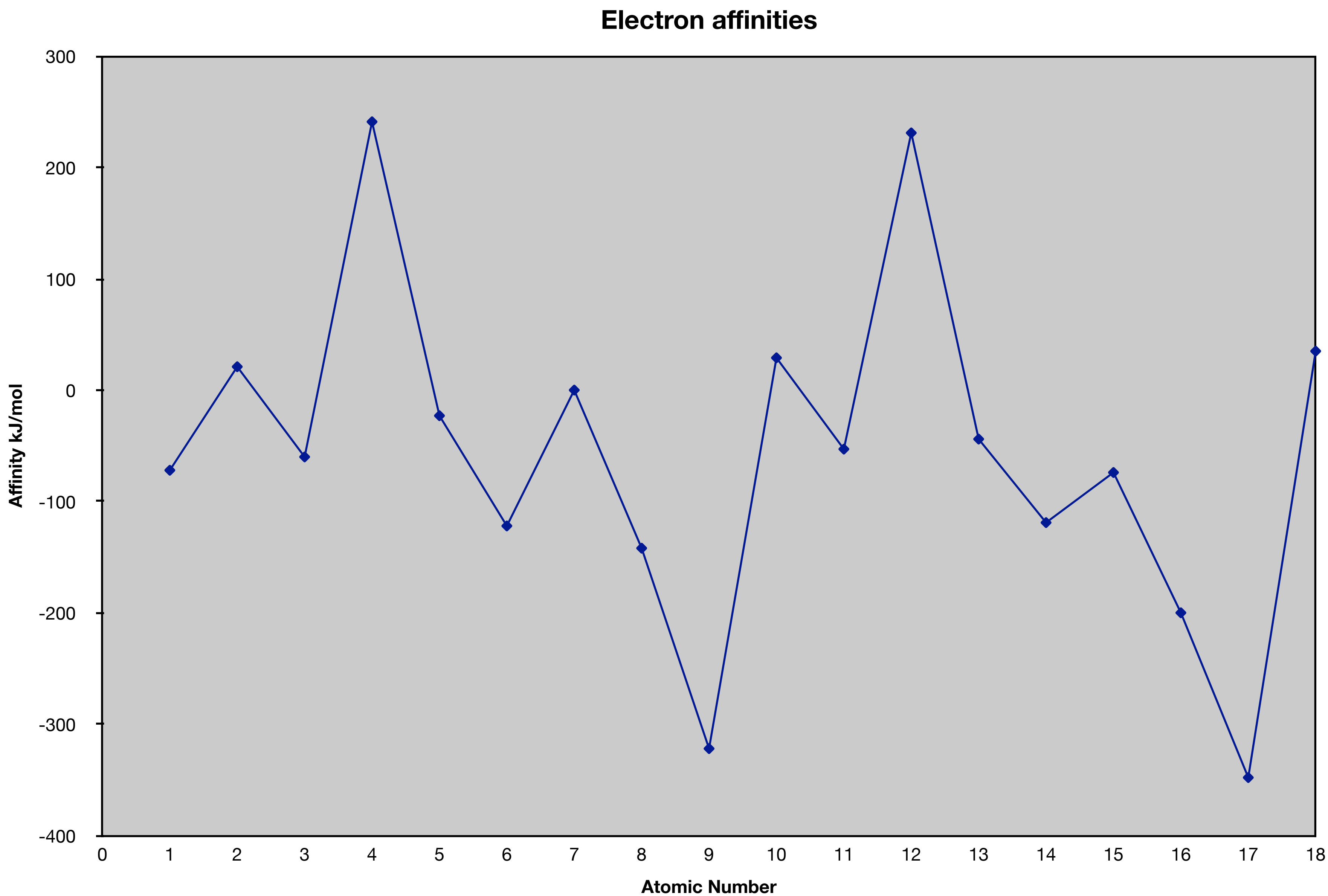

1st Molar Ionization Energy (kJ/mol)
2400
1800
1200
600
0
kJ/mol
0
1
2
3
4
5
6
7
8
Period
Alkalai Metals
Nobel Gases
Chalcogens


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
Atomic Number


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