Periodic Table

First few elements:

H	$1s^1$	↑
He	$1s^2$	(↑↓) ← closed shell
Li	$[He]2s^1$	(↑↓) ↑
Be	$2s^2$	(↑↓) ← but not inert since gap to 2p is small
B	$2s^2 2p^1$	↑
C	$2p^2$	↑ ↑ ← Hund's rule (higher multiplicity tends to have lower energy)
N	$2p^3$	↑ ↑ ↑
O	$2p^4$	↑↓ ↑ ↑
F	$2p^5$	↑↓ ↑↓ ↑
Ne	$2p^6$	(↑↓ ↑↓ ↑↓) ← inert

inert → He; large gap → Li

Ground state determination

What is $^{2S+1}L_J$ of ground state? ← (LS) coupling ($Z \lesssim 30$)
add $\vec{S} = \sum \vec{S}_i$
$\vec{L} = \sum \vec{L}_i$
then $\vec{J} = \vec{L} + \vec{S}$

heavier atoms: (j-j)
$\vec{J}_i = \vec{L}_i + \vec{S}_i$
$\vec{J} = \sum \vec{J}_i$

Hund's rules:

"bus seat" rule

1) couple the valence electrons (or holes) to give maximum total spin
2) choose state of max L (subject to Pauli)
3) if the shell less than half-full ⇒ lowest $J = |L-S|$
   otherwise ⇒ highest $J = L+S$

Justification

Rule 1 & 2: minimize Coulomb interaction between e^-'s

max spin state → symmetric spin part of Ψ_{ground}
(e.g. $|\uparrow\uparrow\rangle$, $|\uparrow\uparrow\uparrow\rangle$ etc.) ⇒ antisymmetric spatial part

← e^- e^- →

⇒ less Coulomb inter.
⇒ lower energy

higher L → electrons "meet" less frequent
⇒ less Coulomb b/w e^-'s

Rule 3: minimize $V_{SO} \propto \langle \hat{L} \cdot \hat{S} \rangle \propto J(J+1) - L(L+S) - S(S+1)$
minimize J (if < half-full)

Ex. B ($Z=5$)
$\{1s^2 2s^2\} 2p^1$ valence e^-

m_ℓ	
1	↑
0	
-1	

$S = \sum m_s = \frac{1}{2}$
$L = \sum m_\ell = 1$
$J = 1/2 \Rightarrow {}^2P_{1/2}$

C ($Z=6$)
$\{1s^2 2s^2\} 2p^2$

m_ℓ	
1	↑
0	↑
-1	

$S = \sum m_s = 1$
$L = \sum m_\ell = 1$
$J = 0 \Rightarrow {}^3P_0$

N (Z=7)
{ } $2p^3$

m_ℓ	
1	↑
0	↑
−1	↑

$S = 3/2$
$L = 0$
$J = 3/2 \Rightarrow {}^4S_{3/2}$

O (Z=8)
{ } $2p^4$
= same as $2p^6 - 2p^2$ (holes)

m_ℓ	
1	↑↓
0	↑
−1	↑

$S = 1$
$L = 1 \Rightarrow {}^3P_2$
$J = 2$ (max)

F (Z=9)
{ } $2p^5 = 2p^6 - 2p^1$ (hole)

m_ℓ	
1	↑↓
0	↑↓
−1	↑

$S = 1/2$
$L = 1 \Rightarrow {}^2P_{3/2}$
$J = 3/2$ (max)

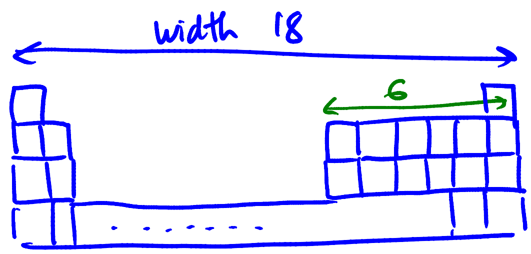
Selection rules (light emission)

electr. dipole : 1) $\Delta J = 0, \pm 1$
($J = 0 \not\leftrightarrow 0$) always forbidden
2) $\Delta m_J = 0, \pm 1$
3) parity of states must change
see HW problem

Elements zoo

	max e^-'s
s :	2
p :	6
d :	10
f :	14

s + p + d = 18



noble gases (18) group
He Ne Ar Kr Xe

[filled shells]
$J = L = S = 0$

* smallest atoms
* self-sufficient (inert)

alkali metals (1)
Li Na K Rb Cs ...

[noble gas filled shell] + ns^1 electron (weakly bound)

* e^- giver! (strongly electropositive)
* largest atoms / soft
* lowest work function

halogens (17)
F Cl Br I ...

[NG] + 1 hole (− electron)

* e^- thief! (strongly electronegative)

alkaline earth metals (2)

Be Mg Ca Sr Ba ...

$[NG] + ns^2$

* like "watered down" version of alkalies (except Be)

transition metals (3-12)

* outer (valence) shell ns^1 or ns^2 electrons (free)
* subshells 3d, 4d, 5d, ... being partially filled (d-d transitions, give vibrant colors to salts)
* many oxidation states: FeO, Fe_3O_4, Fe_2O_3

poor metals (13-16)

Al
Ga
In Sn
Tl Pb Bi

* valence $ns^2 + np^{1,2,3}$
* higher electronegativity than transition metals
* soft, worse conductors

metalloids (13-16)

B
Si
Ge As
Sb Te

* half-filled outer shell
* wierd in-between elements
* semiconductors!

other non-metals (14-16)

C N O
P S
Se

* most abundant in earth's crust
* life stuff!

Lanthanides (rare earth)

↑ 15 each ↓

* filling 4f-subshell
* many hi-tech uses

Actinides

* filling 5f-subshell
* nuclear bomb!