

11/14/2018

## Ch 8 Periodic properties of the elements.

link between QM + PT (periodic table)

Dmitri Mendeleev - late 1860s

- organized known elements into a table.

- organized by atomic mass. (later =  $Z$  atomic #)

insights: (1) chemical props seemed to line-up

(2) Reordered a few elements: Te vs I

(3) Left gaps!!!

127.6 126.9

ex:

	Al	Si	P	S
	27.0	28.0	31.0	32.1
under	eka Al	eka Si	As	Se
			74.9	79.0
predicted missing elements!	In	Sn	Sb	Te
	114.8	118.7	121.8	127.6
	Ga	Ge		

## Gallium (eka-aluminum)



Mendeleev's  
predicted  
properties

Actual  
properties

Atomic mass

About 68 amu

69.72 amu

Melting point

Low

29.8 °C

Density

5.9 g/cm<sup>3</sup>

5.90 g/cm<sup>3</sup>

Formula of oxide

X<sub>2</sub>O<sub>3</sub>

Ga<sub>2</sub>O<sub>3</sub>

Formula of chloride

XCl<sub>3</sub>

GaCl<sub>3</sub>

## Germanium (eka-silicon)



Mendeleev's  
predicted  
properties

Actual  
properties

Atomic mass

About 72 amu

72.64 amu

Density

5.5 g/cm<sup>3</sup>

5.35 g/cm<sup>3</sup>

Formula of oxide

XO<sub>2</sub>

GeO<sub>2</sub>

Formula of chloride

XCl<sub>4</sub>

GeCl<sub>4</sub>



## Electron-configurations: how $e^-$ s occupy orbitals

Basic idea is that  $e^-$ s occupy low E orbitals before higher E orbitals!

(Building-up principle / Auf Bau)

For multi-electron atoms:

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < \dots$   
low E high E

consider H,  $1e^-$   $\#e^-$

$e^-$  config:  $1s^1$   
orbitals

orbital diagram: 1  
1s

arrow refers to  $e^-$  spin:

$m_s = -\frac{1}{2}, +\frac{1}{2}$   
↓      ↑

- write   for each orbital:

$0, \dots, n-1$

$l$	0	1	2	3
code	s	p	d	f

$m_l = -l, \dots, 0, \dots, +l$

$1s$

$n$	$l$	$m_l$
1	0	0

subshell (only one value)

only 1x s-orbital

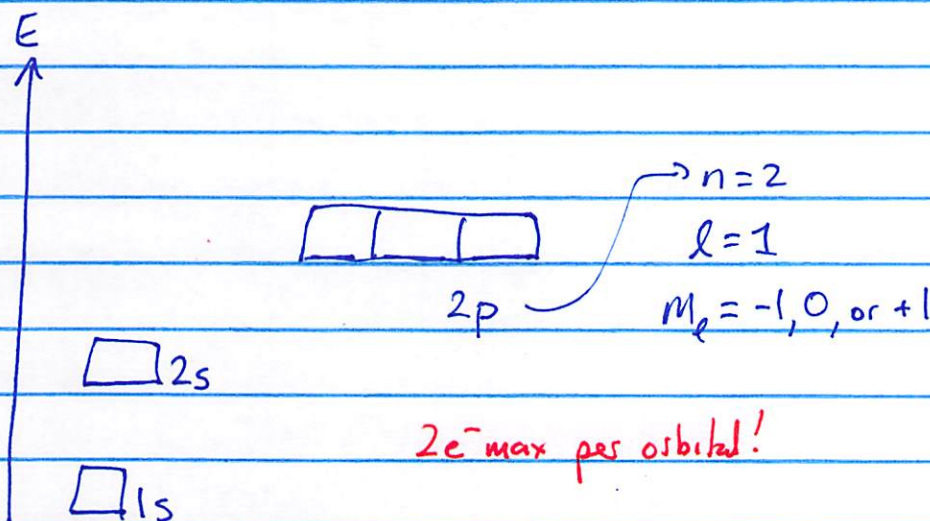
for  ${}^2\text{He}, 2e^-$

$e^-$  config:  $1s^2$

	$n$	$l$	$m_l$	$m_s$
$e^-(1)$	1	0	0	$+\frac{1}{2}$
$e^-(2)$	1	0	0	$-\frac{1}{2}$

orb. diag.  $\boxed{\uparrow\downarrow}$   
 $1s$

Pauli exclusion principle: no two  $e^-$ s are allowed to have same 4 QN in an atom.



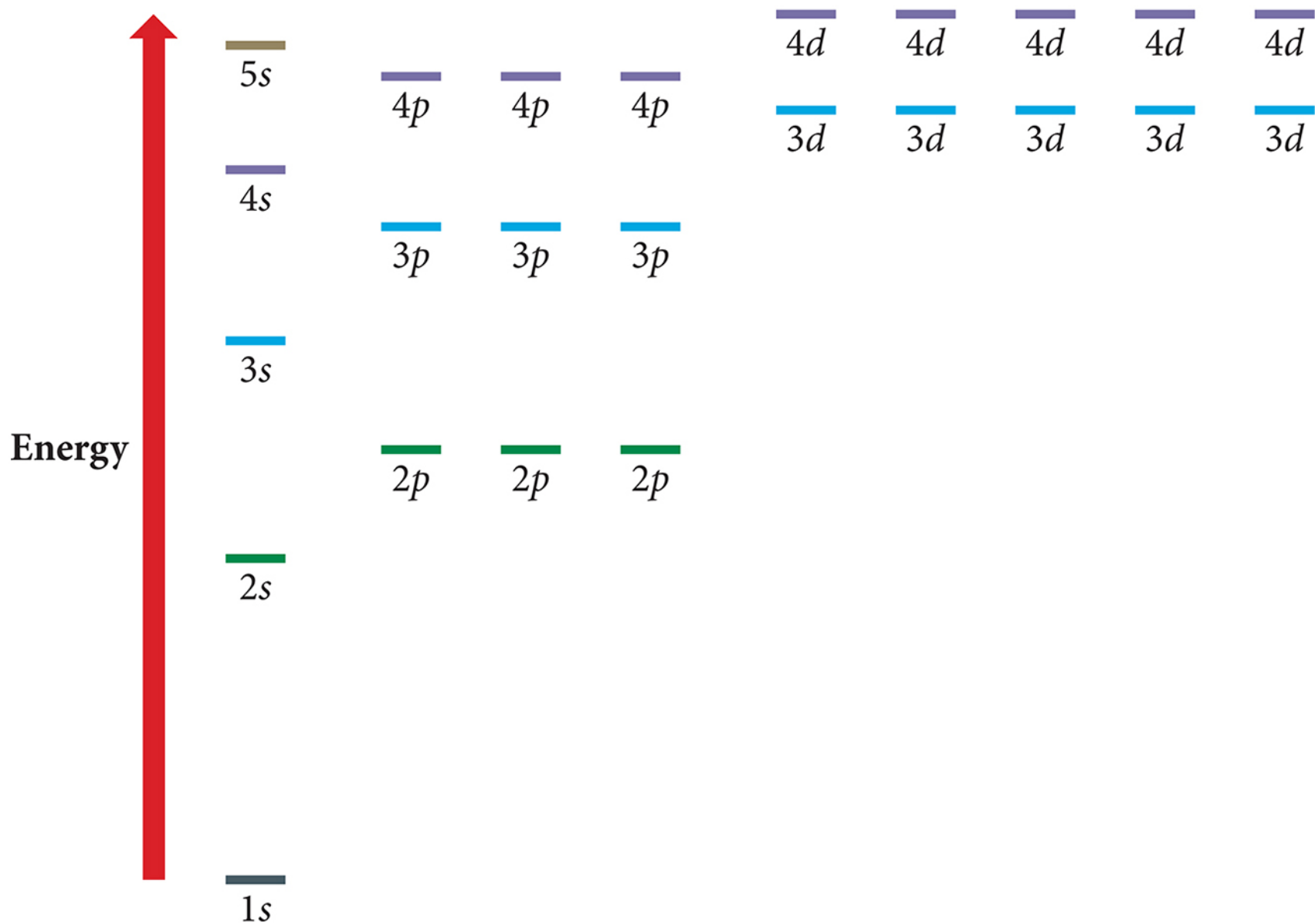
ex:  ${}^3\text{Li}$   $e^-$  config:  $1s^2 2s^1$  orb diag  $\boxed{\uparrow\downarrow}$   $\boxed{\uparrow}$   
 $1s$   $2s$

ex:  ${}^5\text{B}$   $e^-$  config:  $1s^2 2s^2 2p^1$

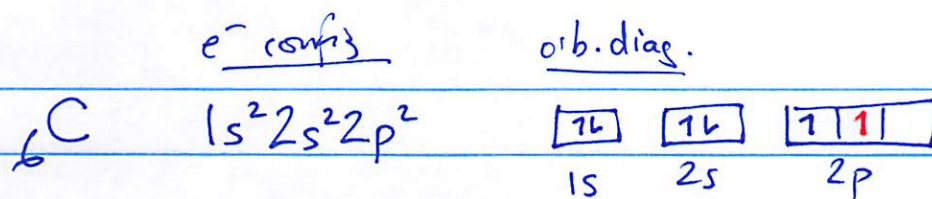
orb diag:  $\boxed{\uparrow\downarrow}$   $\boxed{\uparrow\downarrow}$   $\boxed{\uparrow}$   
 $1s$   $2s$   $2p$

ex:

# General Energy Ordering of Orbitals for Multielectron Atoms

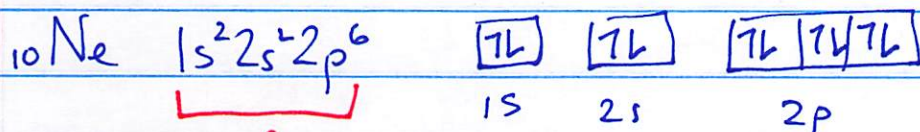
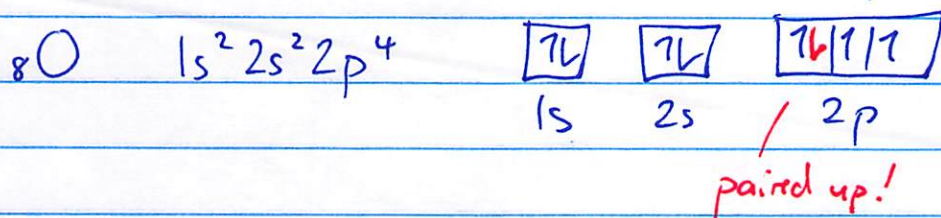




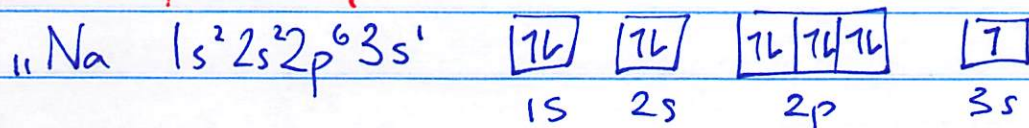


### Hund's rule

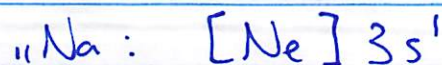
- fill another orbital in subshell w/ parallel spin before pairing up.



same!



can use the noble-gas core abbreviation:



ns  
 princ.  $Q_N$   $l=0: m_l=0$

$\boxed{\uparrow\downarrow}$  :  $2e^-$  max  
 ns

np  $l=1, m_l=-1, 0, +1$

$\boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow}$  :  $6e^-$  max  
 np

nd  $l=2, m_l=-2, -1, 0, +1, +2$

$\boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow}$  :  $10e^-$  max  
 nd

nf  $l=3, m_l=-3, -2, -1, 0, +1, +2, +3$

$\boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow}$  :  $14e^-$  max  
 nf

## Electron configurations, valence $e^-$ s, and the PT

outer  $e^-$ s = valence  $e^-$ s ← used for bonding ←  $e^-$ s in outermost shell (largest  $n$ )

inner  $e^-$ s = core  $e^-$ s

ex: "Na :  $1s^2 2s^2 2p^6 3s^1$   
CORE VALENCE

- we can "read"  $e^-$  configs off of PT.