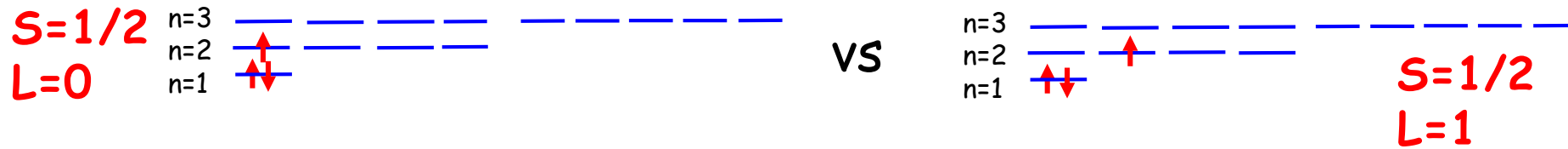
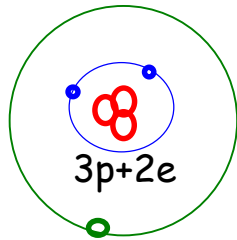


**Rule:** If there is a degeneracy between total  $S=0$  vs total  $S=1$ , the triplet has lower energy due to e-e repulsion.

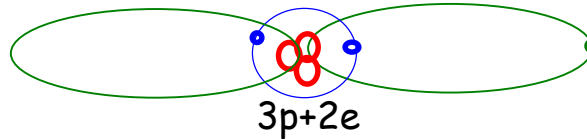
But how do we order states if the degeneracy is between say  $l=0$  vs  $l=1$  for the same  $n$ ? Example:



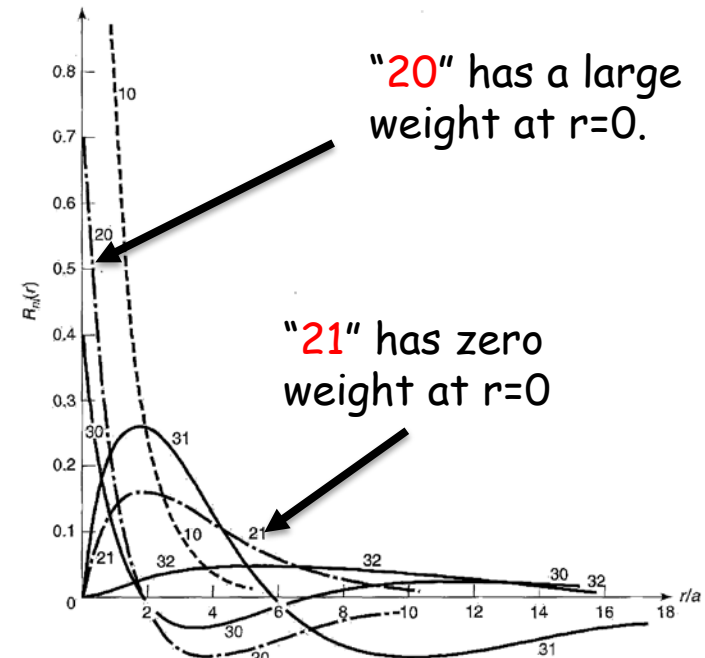
**Rule:** e-p attraction favors the lowest total " $l$ " between subshells (like s vs p) due to "screening" of p:



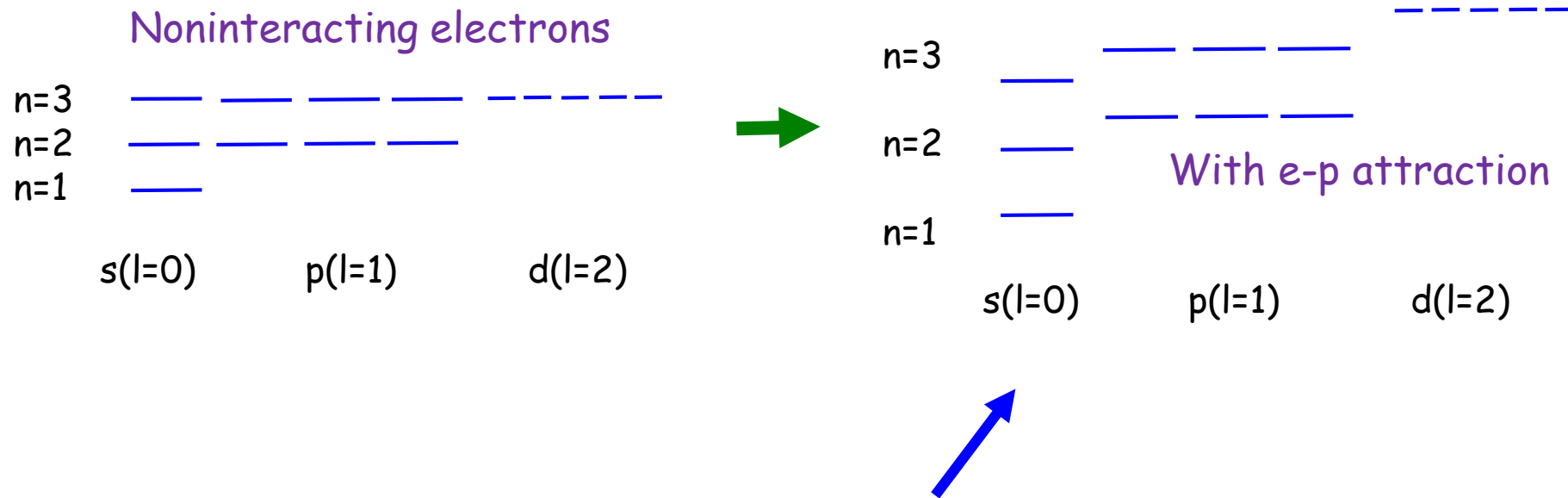
"Green 20" electron is close to nucleus i.e. lower energy. See wave function.



"Green 21" electron is further from nucleus than green 20 electron (screening), see wave function.

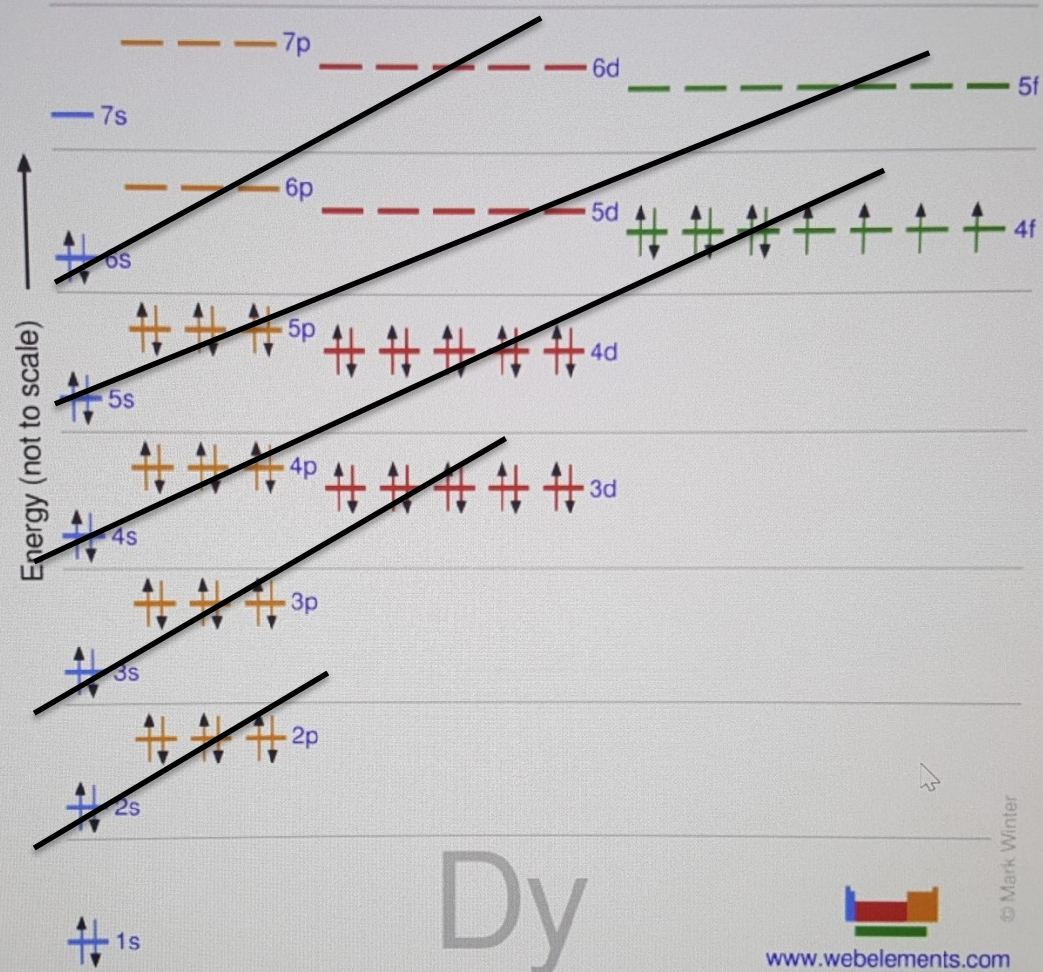


Then, because of the effect in the previous page that distinguishes between cases  $l=0$ ,  $l=1$ ,  $l=2$ , etc. there is a split of accidentally "degenerate" orbitals:



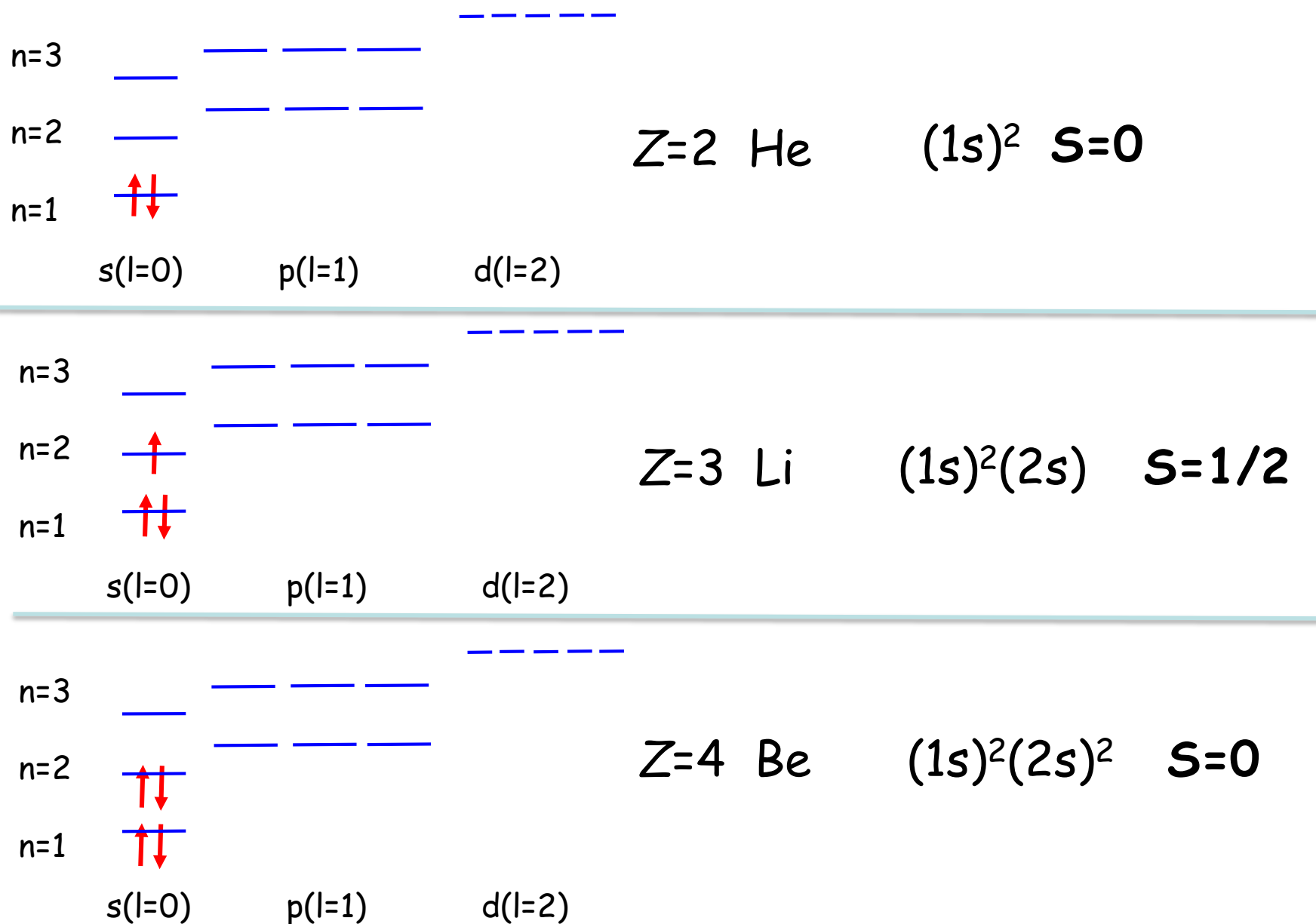
This is the **energy order** we have to use in order to construct the periodic table from now on.

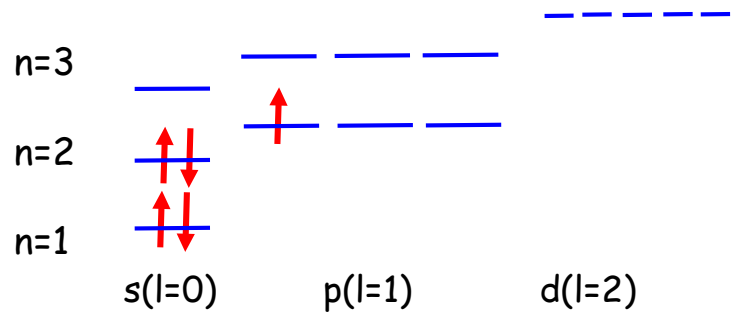
# 8s Dysprosium electronic configuration



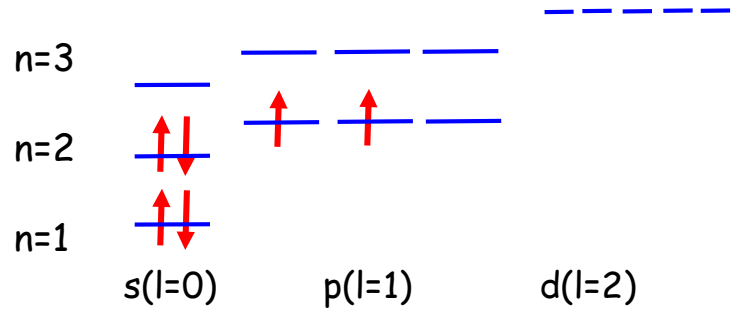
Schematic electronic configuration of dysprosium.

## 5.2.2 Periodic table (ground states only)



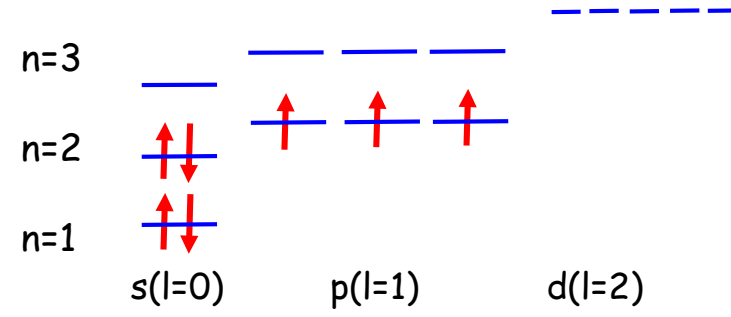


$Z=5$  B  $(1s)^2(2s)^2(2p)$   $S=1/2$



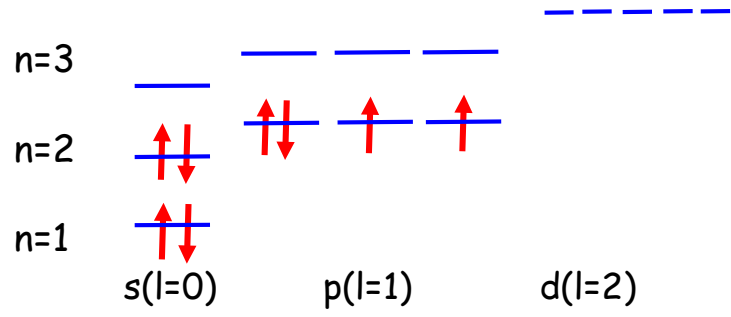
$Z=6$  C  $(1s)^2(2s)^2(2p)^2$   $S=1$

Hund's rule (e-e repulsion,  
as we learned for He)



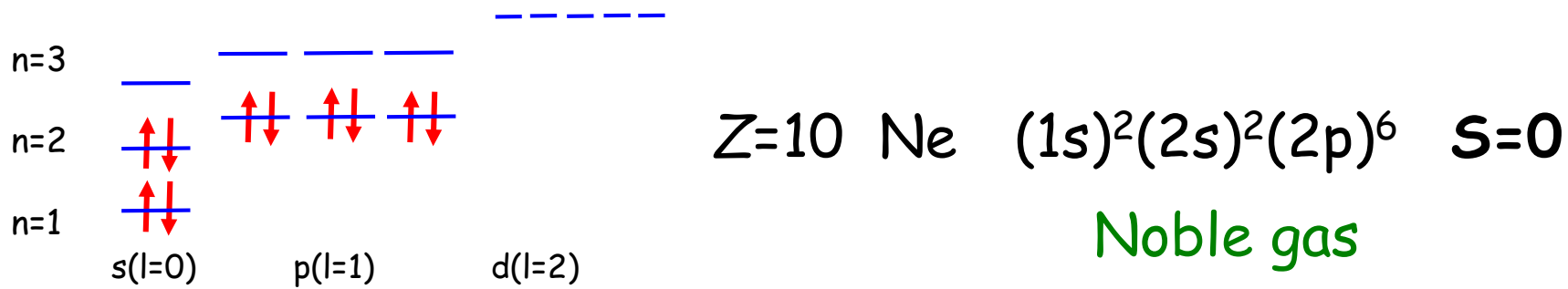
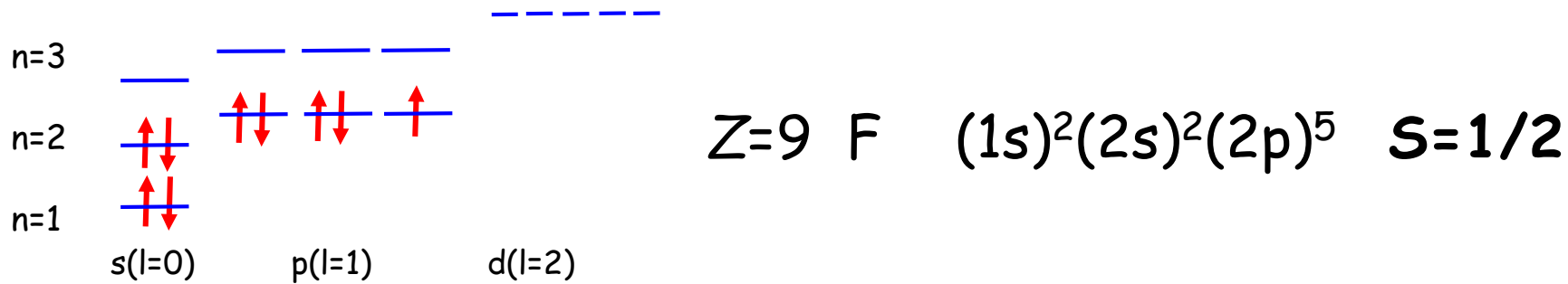
$Z=7$  N  $(1s)^2(2s)^2(2p)^3$   $S=3/2$

Hund's rule (e-e repulsion)



$Z=8$  O  $(1s)^2(2s)^2(2p)^4$   $S=1$

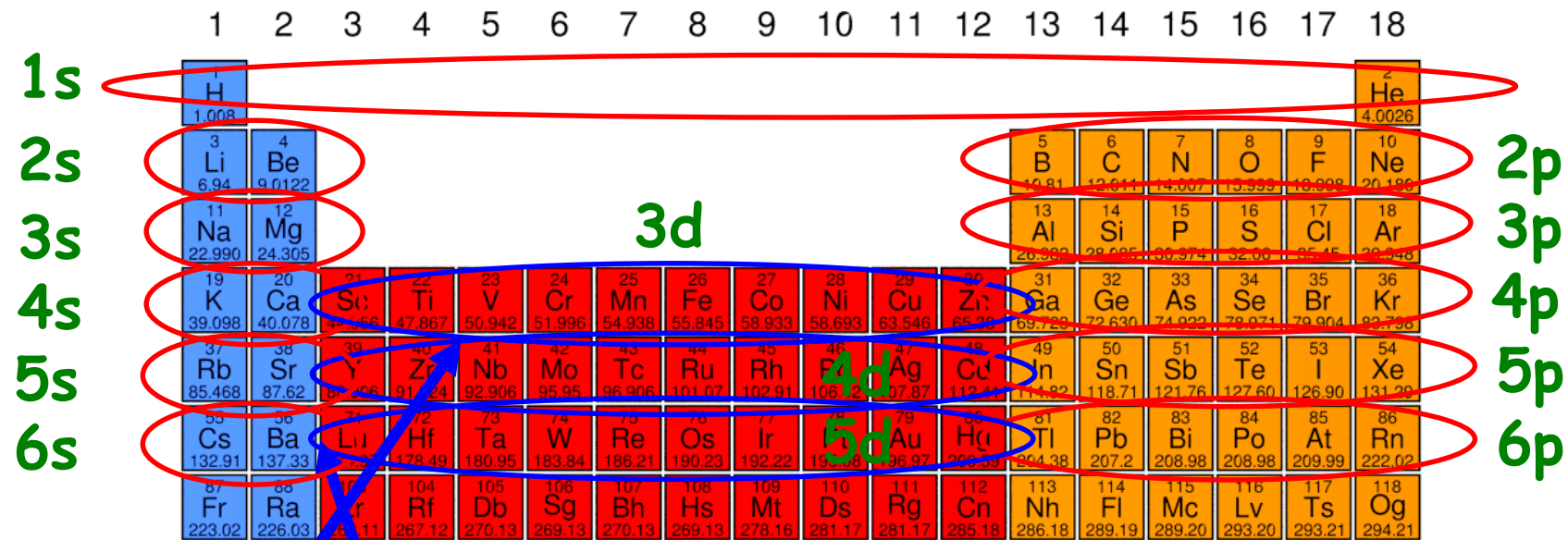
Hund's rule (e-e repulsion)



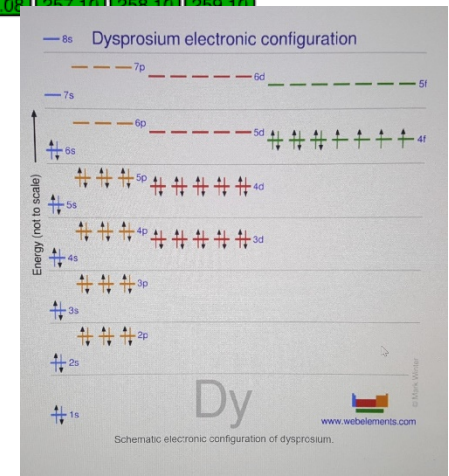
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1 H 1.008	2 He 4.0026																	
3 Li 6.94	4 Be 9.0122																	
11 Na 22.990	12 Mg 24.305																	
19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.867	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.693	29 Cu 63.546	30 Zn 65.38	31 Ga 69.723	32 Ge 72.630	33 As 74.922	34 Se 78.971	35 Br 79.904	36 Kr 83.798	
37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.95	43 Tc 98.906	44 Ru 101.07	45 Rh 106.42	46 Pd 107.57	47 Ag 112.41	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.29	
55 Cs 132.91	56 Ba 137.33	57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm 144.91	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.05	71 Lu 174.96		
87 Fr 223.02	88 Ra 226.03	89 Ac 227.03	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np 237.05	94 Pu 244.06	95 Am 243.06	96 Cm 247.07	97 Bk 247.07	98 Cf 251.08	99 Es 252.08	100 Fm 257.09	101 Md 258.10	102 Lv 260.10	103 Ts 261.10	104 Og 264.10	

Think for a few seconds what we achieved: *the periodic table of Mendeleev*





**Anomaly:** in the split s vs p vs d,  
3d ends up having more energy than 4s



S

Z	Element	Configuration	S
1	H	(1s)	1/2 <sup>2</sup> S <sub>1/2</sub>
2	He	(1s) <sup>2</sup>	0 <sup>1</sup> S <sub>0</sub>
3	Li	(He)(2s)	1/2 <sup>2</sup> S <sub>1/2</sub>
4	Be	(He)(2s) <sup>2</sup>	0 <sup>1</sup> S <sub>0</sub>
5	B	(He)(2s) <sup>2</sup> (2p)	1/2 <sup>2</sup> P <sub>1/2</sub>
6	C	(He)(2s) <sup>2</sup> (2p) <sup>2</sup>	1 <sup>3</sup> P <sub>0</sub>
7	N	(He)(2s) <sup>2</sup> (2p) <sup>3</sup>	3/2 <sup>4</sup> S <sub>3/2</sub>
8	O	(He)(2s) <sup>2</sup> (2p) <sup>4</sup>	1 <sup>3</sup> P <sub>2</sub>
9	F	(He)(2s) <sup>2</sup> (2p) <sup>5</sup>	1/2 <sup>2</sup> P <sub>3/2</sub>
10	Ne	(He)(2s) <sup>2</sup> (2p) <sup>6</sup>	0 <sup>1</sup> S <sub>0</sub>
11	Na	(Ne)(3s)	1/2 <sup>2</sup> S <sub>1/2</sub>
12	Mg	(Ne)(3s) <sup>2</sup>	0 <sup>1</sup> S <sub>0</sub>
13	Al	(Ne)(3s) <sup>2</sup> (3p)	1/2 <sup>2</sup> P <sub>1/2</sub>
14	Si	(Ne)(3s) <sup>2</sup> (3p) <sup>2</sup>	1 <sup>3</sup> P <sub>0</sub>
15	P	(Ne)(3s) <sup>2</sup> (3p) <sup>3</sup>	3/2 <sup>4</sup> S <sub>3/2</sub>
16	S	(Ne)(3s) <sup>2</sup> (3p) <sup>4</sup>	1 <sup>3</sup> P <sub>2</sub>
17	Cl	(Ne)(3s) <sup>2</sup> (3p) <sup>5</sup>	1/2 <sup>2</sup> P <sub>3/2</sub>
18	Ar	(Ne)(3s) <sup>2</sup> (3p) <sup>6</sup>	0 <sup>1</sup> S <sub>0</sub>

$$2S+1L_J$$

All 3 numbers are TOTAL  
 In each subshell, like 2p, the state with max S total, wins. Example: N has 2S+1=4 i.e. S=3/2 due to e-e repulsion.

About L: "S" means L=0, "P" means L=1, "D" means L=2, ..., but now L is "total L".

J, the total angular momentum, could be L+S, ..., |L-S| depending on small energy differences.

The "Hund's rules" for L and J are more chaotic, with many exceptions. Just read about them in the book if you like ...



Up to this point is what you need to know for Test 1.

**One problem will surely involve the diagonalization of a  $2 \times 2$  matrix in the context of a spin in a magnetic field.**