I. Periodic Table

- Schrödinger Equation + Independent Particle Approximation (→ atomic orbitals)

  \+ Pauli Exclusion Principle

  Explain much physics of atoms and the periodic table

- Ground state:

  fill electrons into atomic orbitals according to Pauli Exclusion Principle

			Ti = 50	Zr = 90	? = 180.
			V = 51	Nb = 94	Ta = 182.
			Cr = 52	Mo = 96	W = 186.
			Mn = 55	Rh = 104,4	Pt = 197,4
			Fe = 56	Ru = 104,4	Ir = 198.
			Ni = Co = 59	Pl = 106,6	Os = 199.
H = 1			Cu = 63,4	Ag = 108	Hg = 200.
	Be = 9,4	Mg = 24	Zn = 65,2	Cd = 112	
	B = 11	Al = 27,4	? = 68	Ur = 116	Au = 197?
	C = 12	Si = 28	? = 70	Sn = 118	
	N = 14	P = 31	As = 75	Sb = 122	Bi = 210?
	O = 16	S = 32	Se = 79,4	Te = 128?	
	F = 19	Cl = 35,5	Br = 80	J = 127	
Li = 7	Na = 23	K = 39	Rb = 85,4	Cs = 133	Tl = 204.
		Ca = 40	Sr = 87,6	Ba = 137	Pb = 207.
		? = 45	Ce = 92		
		? Er = 56	La = 94		
		? Yt = 60	Di = 95		
		? In = 75,6	Th = 118?		

Д. Менделеев.

Mendeleev's original February 1869 publication of his short-form periodic system, entitled "An Attempt at a System of Elements, Based on Their Atomic Weight and Chemical Affinity."

Mendeleev 1869 version

2019 is the International Year of the Periodic Table (as declared by the United Nations)

IUPAC Periodic Table of the Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 **H** hydrogen 1.008 [1.0078, 1.0082]																	2 **He** helium 4.0026
3 **Li** lithium 6.94 [6.938, 6.997]	4 **Be** beryllium 9.0122											5 **B** boron 10.81 [10.806, 10.821]	6 **C** carbon 12.011 [12.009, 12.012]	7 **N** nitrogen 14.007 [14.006, 14.008]	8 **O** oxygen 15.999 [15.999, 16.000]	9 **F** fluorine 18.998	10 **Ne** neon 20.180
11 **Na** sodium 22.990	12 **Mg** magnesium 24.305 [24.304, 24.307]											13 **Al** aluminium 26.982	14 **Si** silicon 28.085 [28.084, 28.086]	15 **P** phosphorus 30.974	16 **S** sulfur 32.06 [32.059, 32.076]	17 **Cl** chlorine 35.45 [35.446, 35.457]	18 **Ar** argon 39.95 [39.792, 39.963]
19 **K** potassium 39.098	20 **Ca** calcium 40.078(4)	21 **Sc** scandium 44.956	22 **Ti** titanium 47.867	23 **V** vanadium 50.942	24 **Cr** chromium 51.996	25 **Mn** manganese 54.938	26 **Fe** iron 55.845(2)	27 **Co** cobalt 58.933	28 **Ni** nickel 58.693	29 **Cu** copper 63.546(3)	30 **Zn** zinc 65.38(2)	31 **Ga** gallium 69.723	32 **Ge** germanium 72.630(8)	33 **As** arsenic 74.922	34 **Se** selenium 78.971(8)	35 **Br** bromine 79.904 [79.901, 79.907]	36 **Kr** krypton 83.798(2)
37 **Rb** rubidium 85.468	38 **Sr** strontium 87.62	39 **Y** yttrium 88.906	40 **Zr** zirconium 91.224(2)	41 **Nb** niobium 92.906	42 **Mo** molybdenum 95.95	43 **Tc** technetium	44 **Ru** ruthenium 101.07(2)	45 **Rh** rhodium 102.91	46 **Pd** palladium 106.42	47 **Ag** silver 107.87	48 **Cd** cadmium 112.41	49 **In** indium 114.82	50 **Sn** tin 118.71	51 **Sb** antimony 121.76	52 **Te** tellurium 127.60(3)	53 **I** iodine 126.90	54 **Xe** xenon 131.29
55 **Cs** caesium 132.91	56 **Ba** barium 137.33	57-71 lanthanoids	72 **Hf** hafnium 178.49(2)	73 **Ta** tantalum 180.95	74 **W** tungsten 183.84	75 **Re** rhenium 186.21	76 **Os** osmium 190.23(3)	77 **Ir** iridium 192.22	78 **Pt** platinum 195.08	79 **Au** gold 196.97	80 **Hg** mercury 200.59	81 **Tl** thallium 204.38 [204.38, 204.39]	82 **Pb** lead 207.2	83 **Bi** bismuth 208.98	84 **Po** polonium	85 **At** astatine	86 **Rn** radon
87 **Fr** francium	88 **Ra** radium	89-103 actinoids	104 **Rf** rutherfordium	105 **Db** dubnium	106 **Sg** seaborgium	107 **Bh** bohrium	108 **Hs** hassium	109 **Mt** meitnerium	110 **Ds** darmstadtium	111 **Rg** roentgenium	112 **Cn** copernicium	113 **Nh** nihonium	114 **Fl** flerovium	115 **Mc** moscovium	116 **Lv** livermorium	117 **Ts** tennessine	118 **Og** oganesson

Key:

atomic number **Symbol** **name** conventional atomic weight standard atomic weight

57 **La** lanthanum 138.91	58 **Ce** cerium 140.12	59 **Pr** praseodymium 140.91	60 **Nd** neodymium 144.24	61 **Pm** promethium	62 **Sm** samarium 150.36(2)	63 **Eu** europium 151.96	64 **Gd** gadolinium 157.25(3)	65 **Tb** terbium 158.93	66 **Dy** dysprosium 162.50	67 **Ho** holmium 164.93	68 **Er** erbium 167.26	69 **Tm** thulium 168.93	70 **Yb** ytterbium 173.05	71 **Lu** lutetium 174.97
89 **Ac** actinium	90 **Th** thorium 232.04	91 **Pa** protactinium 231.04	92 **U** uranium 238.03	93 **Np** neptunium	94 **Pu** plutonium	95 **Am** americium	96 **Cm** curium	97 **Bk** berkelium	98 **Cf** californium	99 **Es** einsteinium	100 **Fm** fermium	101 **Md** mendelevium	102 **No** nobelium	103 **Lr** lawrencium

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

For notes and updates to this table, see www.iupac.org. This version is dated 1 December 2018.

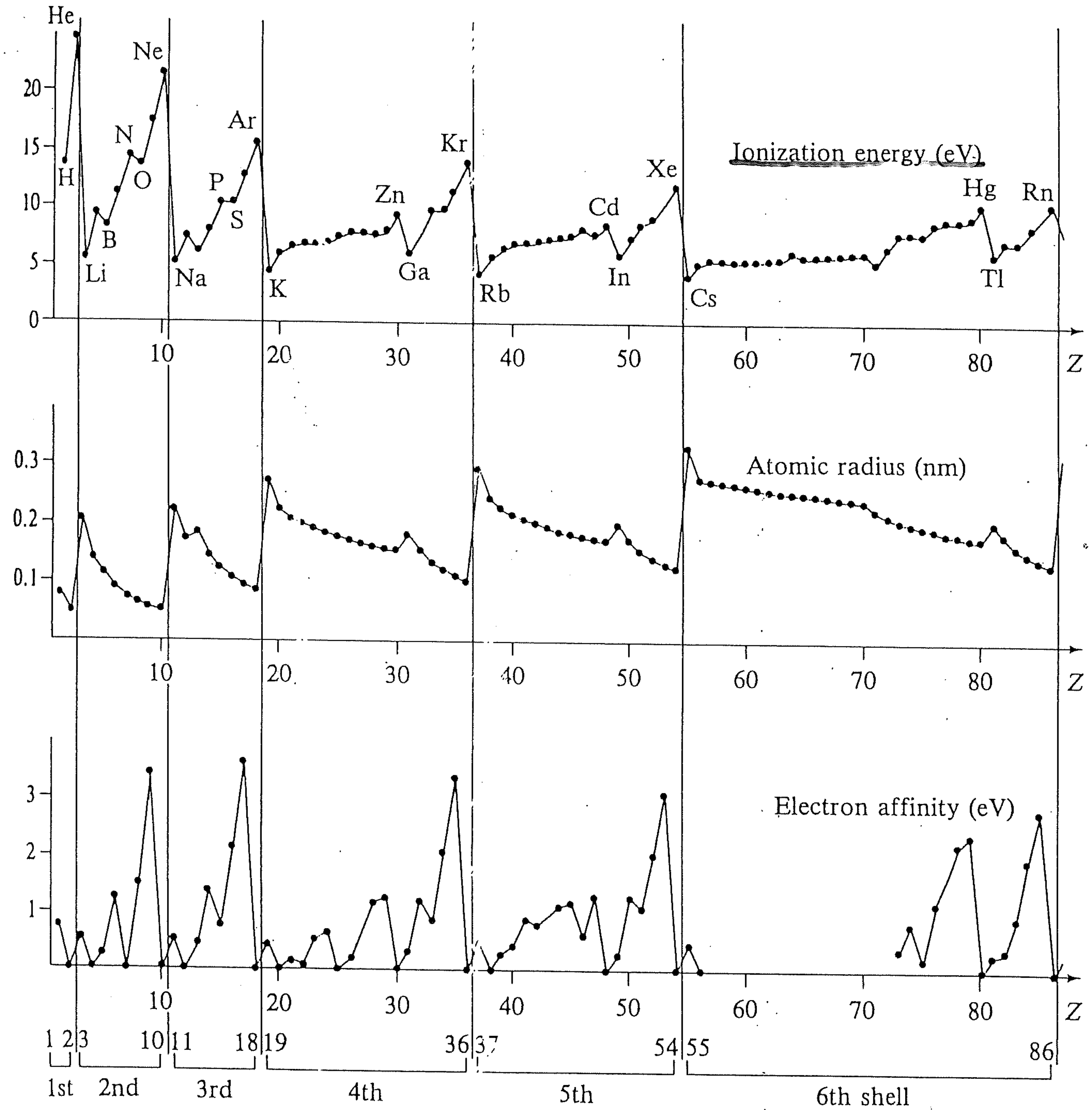
United Nations
Educational, Scientific and
Cultural Organization

International Year
of the Periodic Table
of Chemical Elements

1 December 2018 version (latest)

AP-VIII-3

Periodicity in physical properties of elements



Ionization energy, atomic radius, and electron affinity as functions of atomic number Z. The vertical lines separate complete shells. The electron affinities for elements 57 through 72 have not been measured.

Electronic Configurations of the Elements

Z	Symbol	Ground Configuration	Ionization Energy (eV)
1	H	$1s^1$	13.595
2	He	$1s^2$	24.581
3	Li	[He] $2s^1$	5.390
4	Be	$2s^2$	9.320
5	B	$2s^22p^1$	8.296
6	C	$2s^22p^2$	11.256
7	N	$2s^22p^3$	14.545
8	O	$2s^22p^4$	13.614
9	F	$2s^22p^5$	17.418
10	Ne	$2s^22p^6$	21.559
11	Na	[Ne] $3s^1$	5.138
12	Mg	$3s^2$	7.644
13	Al	$3s^23p^1$	5.984
14	Si	$3s^23p^2$	8.149
15	P	$3s^23p^3$	10.484
16	S	$3s^23p^4$	10.357
17	Cl	$3s^23p^5$	13.01
18	Ar	$3s^23p^6$	15.755
19	K	[Ar] $4s^1$	4.339
20	Ca	$4s^2$	6.111
21	Sc	$3d4s^2$	6.54
22	Ti	$3d^24s^2$	6.83
23	V	$3d^34s^2$	6.74
24	Cr	$3d^54s$	6.76
25	Mn	$3d^54s^2$	7.432
26	Fe	$3d^64s^2$	7.87
27	Co	$3d^74s^2$	7.86
28	Ni	$3d^84s^2$	7.633
29	Cu	$3d^{10}4s^1$	7.724
30	Zn	$3d^{10}4s^2$	9.391
31	Ga	$3d^{10}4s^24p^1$	6.00
32	Ge	$3d^{10}4s^24p^2$	7.88
33	As	$3d^{10}4s^24p^3$	9.81
34	Se	$3d^{10}4s^24p^4$	9.75
35	Br	$3d^{10}4s^24p^5$	11.84
36	Kr	$3d^{10}4s^24p^6$	13.996
37	Rb	[Kr] $5s^1$	4.176
38	Sr	$5s^2$	5.692
39	Y	$4d5s^2$	6.377
40	Zr	$4d^25s^2$	6.835
41	Nb	$4d^45s^1$	6.881
42	Mo	$4d^55s^1$	7.10
43	Tc	$4d^55s^2$	7.228
44	Ru	$4d^75s^1$	7.365
45	Rh	$4d^85s^1$	7.461
46	Pd	$4d^{10}$	8.33
47	Ag	$4d^{10}5s^1$	7.574
48	Cd	$4d^{10}5s^2$	8.991
49	In	$4d^{10}5s^25p^1$	5.785
50	Sn	$4d^{10}5s^25p^2$	7.342
51	Sb	$4d^{10}5s^25p^3$	8.639
52	Te	$4d^{10}5s^25p^4$	9.01

[From Serway et al., "Modern Physics"]

Cont'd

Z	Symbol	Ground Configuration	Ionization Energy (eV)
53	I	$4d^{10}5s^25p^5$	10.454
54	Xe	$4d^{10}5s^25p^6$	12.127
55	Cs	[Xe] $6s^1$	3.893
56	Ba	$6s^2$	5.210
57	La	$5d6s^2$	5.61
58	Ce	$4f5d6s^2$	6.54
59	Pr	$4f^36s^2$	5.48
60	Nd	$4f^46s^2$	5.51
61	Pm	$4f^56s^2$	
62	Fm	$4f^66s^2$	5.6
63	Eu	$4f^76s^2$	5.67
64	Gd	$4f^75d6s^2$	6.16
65	Tb	$4f^96s^2$	6.74
66	Dy	$4f^{10}6s^2$	6.82
67	Ho	$4f^{11}6s^2$	
68	Er	$4f^{12}6s^2$	
69	Tm	$4f^{13}6s^2$	
70	Yb	$4f^{14}6s^2$	6.22
71	Lu	$4f^{14}5d6s^2$	6.15
72	Hf	$4f^{14}5d^26s^2$	7.0
73	Ta	$4f^{14}5d^36s^2$	7.88
74	W	$4f^{14}5d^46s^2$	7.98
75	Re	$4f^{14}5d^56s^2$	7.87
76	Os	$4f^{14}5d^66s^2$	8.7
77	Ir	$4f^{14}5d^76s^2$	9.2
78	Pt	$4f^{14}5d^86s^2$	8.88

Z	Symbol	Ground Configuration	Ionization Energy (eV)
79	Au	[Xe, $4f^{14}5d^{10}$] $6s^1$	9.22
80	Hg	$6s^2$	10.434
81	Tl	$6s^26p^1$	6.106
82	Pb	$6s^26p^2$	7.415
83	Bi	$6s^26p^3$	7.287
84	Po	$6s^26p^4$	8.43
85	At	$6s^26p^5$	
86	Rn	$6s^26p^6$	10.745
87	Fr	[Rn] $7s^1$	
88	Ra	$7s^2$	5.277
89	Ac	$6d7s^2$	6.9
90	Th	$6d^27s^2$	
91	Pa	$5f^26d7s^2$	
92	U	$5f^36d7s^2$	4.0
93	Np	$5f^46d7s^2$	
94	Pu	$5f^67s^2$	
95	Am	$5f^77s^2$	
96	Cm	$5f^76d7s^2$	
97	Bk	$5f^86d7s^2$	
98	Cf	$5f^{10}7s^2$	
99	Es	$5f^{11}7s^2$	
100	Fm	$5f^{12}7s^1$	
101	Mv	$5f^{13}7s^2$	
102	No	$5f^{14}7s^2$	
103	Lw	$5f^{14}6d7s^2$	
104	Ku	$5f^{14}6d^27s^2$	

Note: The bracket notation is used as a shorthand method to avoid repetition in indicating inner shell electrons. Thus, [He] represents $1s^2$, [Ne]represents $1s^22s^22p^6$, [Ar] represents $1s^22s^22p^63s^23p^6$, and so on.

Lithium (Z=3)

2s — ↑ — ← can be up or down

1s — ↑↓ — [filled "1s shell" (or closed shell)]

"spins cancelled" in closed shell

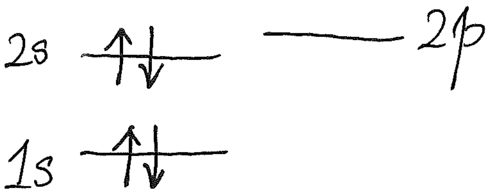
- 1s electrons are tightly bound
  - 1s electrons: not involved in chemistry
  - tightly bound: see Z = 3 (+3e nucleus)
- 2s electron is much less tightly bound (screening effect of 1s electrons)

  ⇒ easier to set the 2s electron free

  ↳ smaller ionization energy (~5.4 eV) than H and He atoms

  ionization energy: energy to turn lithium atom into Li^+ ion.
- $1s^2\,2s^1$ Term Symbol: $^2S_{1/2}$ (for $^{2S+1}L_J$)

Beryllium (Z = 4)



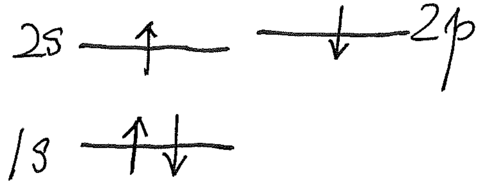
Ground state

- Term Symbol

$^{1}S_{0}$

All spins paired up

- $S = 0 \Rightarrow 2S+1 = 1$ (superscript)
- s-states involved ($L = 0$, thus S)
- $J = 0$ (subscript)



(schematic)

First excited state

- don't need much energy to excite (2.7 eV) to first excited state
- The lonely 2p and 2s electrons can form chemical bonds with other atoms (gain energy back)

∴ Chemically active

Boron to Neon ($Z=5$ to $Z=10$) [filling 2p states]

- Boron ($Z=5$): $1s^2\ 2s^2\ 2p^1$ Term Symbol: ${}^2P_{1/2}$

$1s^2 2s^2 2p^1 \rightarrow$ B, C, N, O, F, Ne $\leftarrow 1s^2 2s^2 2p^6$

- Florine ($Z=9$): F^- ion has $2p^6$ closed shell structure

F^- ion has lower energy than F atom!

$\Rightarrow$ give out energy when F catches an electron to form F^-

(give out energy = electron affinity) [3.4 eV for Florine]

Quantum Mechanically, need to do two calculations (one for F, one for F^-) to get electron affinity

(different Hamiltonians)

Aside: What to learn in more advanced Atomic Physics Courses?

Carbon: $1s^2\ 2s^2\ 2p^2$

2p — — — — — — $m_\ell = 1, 0, -1$
$m_s = +1/2, -1/2$

How to put two electrons to achieve lowest energy?

[there are $15 = \frac{6!}{2!4!}$ ways, which has lowest energy?]

Idea: $\hat{H}_{atom} \neq IPA$

difference becomes perturbation

results summarized as Hund's rules

The Other Elements

Electron configurations of the ground states of the first 18 elements.

First shell		Second shell		Third shell	
$_1H$:	$1s^1$	$_3Li$:	$1s^2 2s^1$	$_{11}Na$:	$1s^2 2s^2 2p^6 3s^1$
$_2He$:	$1s^2$	$_4Be$:	$1s^2 2s^2$	$_{12}Mg$:	$1s^2 2s^2 2p^6 3s^2$
		$_5B$:	$1s^2 2s^2 2p^1$	$_{13}Al$:	$1s^2 2s^2 2p^6 3s^2 3p^1$
		$_6C$:	$1s^2 2s^2 2p^2$	$_{14}Si$:	$1s^2 2s^2 2p^6 3s^2 3p^2$
		$_7N$:	$1s^2 2s^2 2p^3$	$_{15}P$:	$1s^2 2s^2 2p^6 3s^2 3p^3$
		$_8O$:	$1s^2 2s^2 2p^4$	$_{16}S$:	$1s^2 2s^2 2p^6 3s^2 3p^4$
		$_9F$:	$1s^2 2s^2 2p^5$	$_{17}Cl$:	$1s^2 2s^2 2p^6 3s^2 3p^5$
		$_{10}Ne$:	$1s^2 2s^2 2p^6$	$_{18}Ar$:	$1s^2 2s^2 2p^6 3s^2 3p^6$

Potassium (Z = 19)

19th electron → 3d or 4s ?

have to do a QM calculation

turns out 4s level is slightly lower in energy

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$

[The outer electrons are usually referred to as the valence electrons. (價電子)

They govern the valence, e.g. K^+, and hence the chemistry.]

Calcium (Z = 20)

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$

Transition Metals (Filling in 3d states (10 of them))

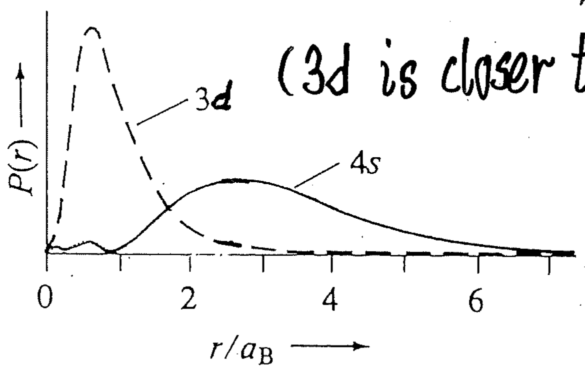
Sc Ti V Cr Mn Fe Co Ni Cu Zn

They have similarities.

Why?

- Chemistry is usually determined by the outer (4s) electrons

(3d is closer to nucleus)



Typical radial probability distributions for a $3d$ and $4s$ electron in the transition elements $_{21}Sc$ through $_{30}Zn$. Note how the $4s$ distribution peaks more than four times farther out than the $3d$. For this reason it is the $4s$ electrons that determine the chemical properties of the transition metals.

- Transition Metals differ only in number of 3d electrons
  ⇒ they have similar chemical properties

3d elements are important magnetic materials

- How to fill in 5 electrons in d-orbitals?

e.g. $3d^5$

	↑	↑	↑	↑	↑
($l=2$) [d states] m_l:	-2	-1	0	$+1$	$+2$

← Maximize the total spin S quantum number as allowed by Pauli Principle

[as many parallel spins are possible]

This is Hund's rule (Hund's rule #1)

(Hund's rule: "rules" summarizing results of many QM calculations)

- This is how some atoms acquire a NET magnetic dipole moment
- When magnetic moments of different atoms tend to align (at low temperature), we have ferromagnetism (note: originated from spin & exchange integral)

After the transition metals,

Ga Ge As Se Br Kr ($Z=36$) fill up 4p states

(Ga, Ge, As, Se: important elements in semiconductor physics/industry)

- Si, Ge (elemental semiconductors)
- GaAs, InP (compound III-V semiconductors)
- HgTe, CdTe, CdSe (compound II-VI semiconductors)

Summary

- Quantum Mechanics is key to understand atoms
- Atomic orbitals resulted from reducing (approximating) many-electron problem to single-electron problem
- Pauli Exclusion Principle is a consequence of anti-symmetric requirement of many-electron wavefunctions
- Atomic Orbitals + Pauli Exclusion Principle (both are QM results) explain much physics of atoms and the periodic table

  [physics unaccounted for by IPA gives further details]