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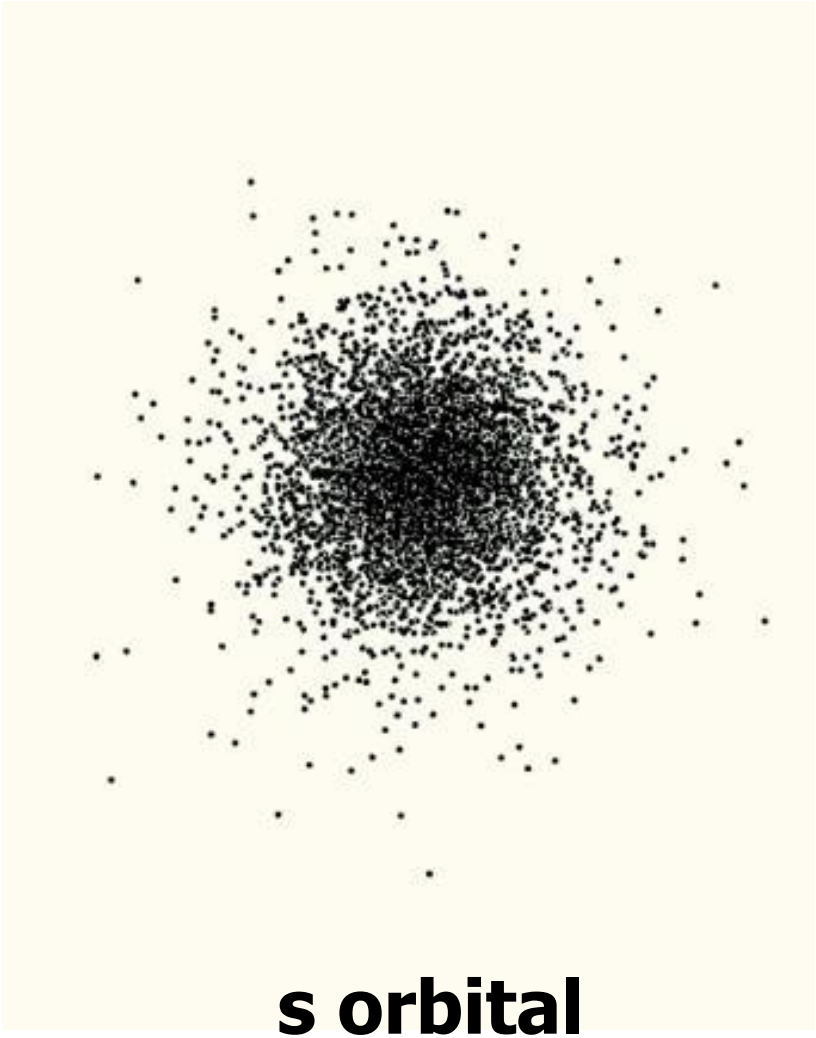
ELECTRON ARRANGEMENT

Shells, sub-shells & orbitals

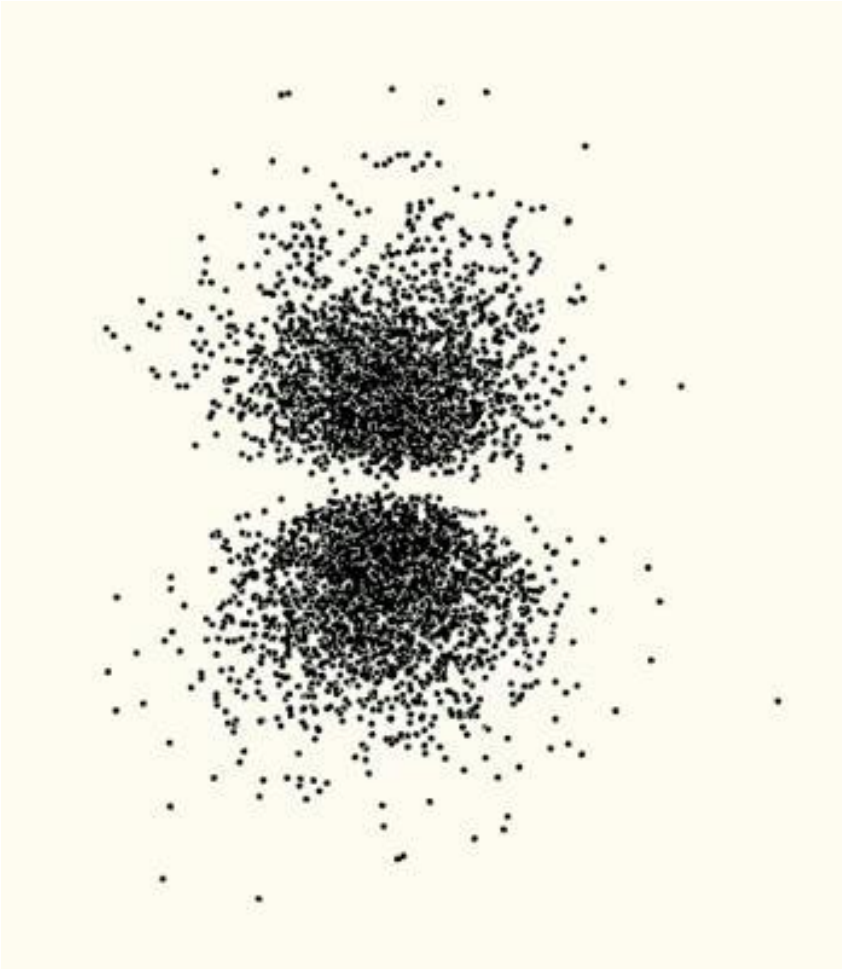
- Electrons are arranged in electrons shells (energy levels).
- The shells have sub-shells (sub-levels).
- Each shell/sub-shell is made up of electron orbitals which can each hold 2 electrons.

Orbitals

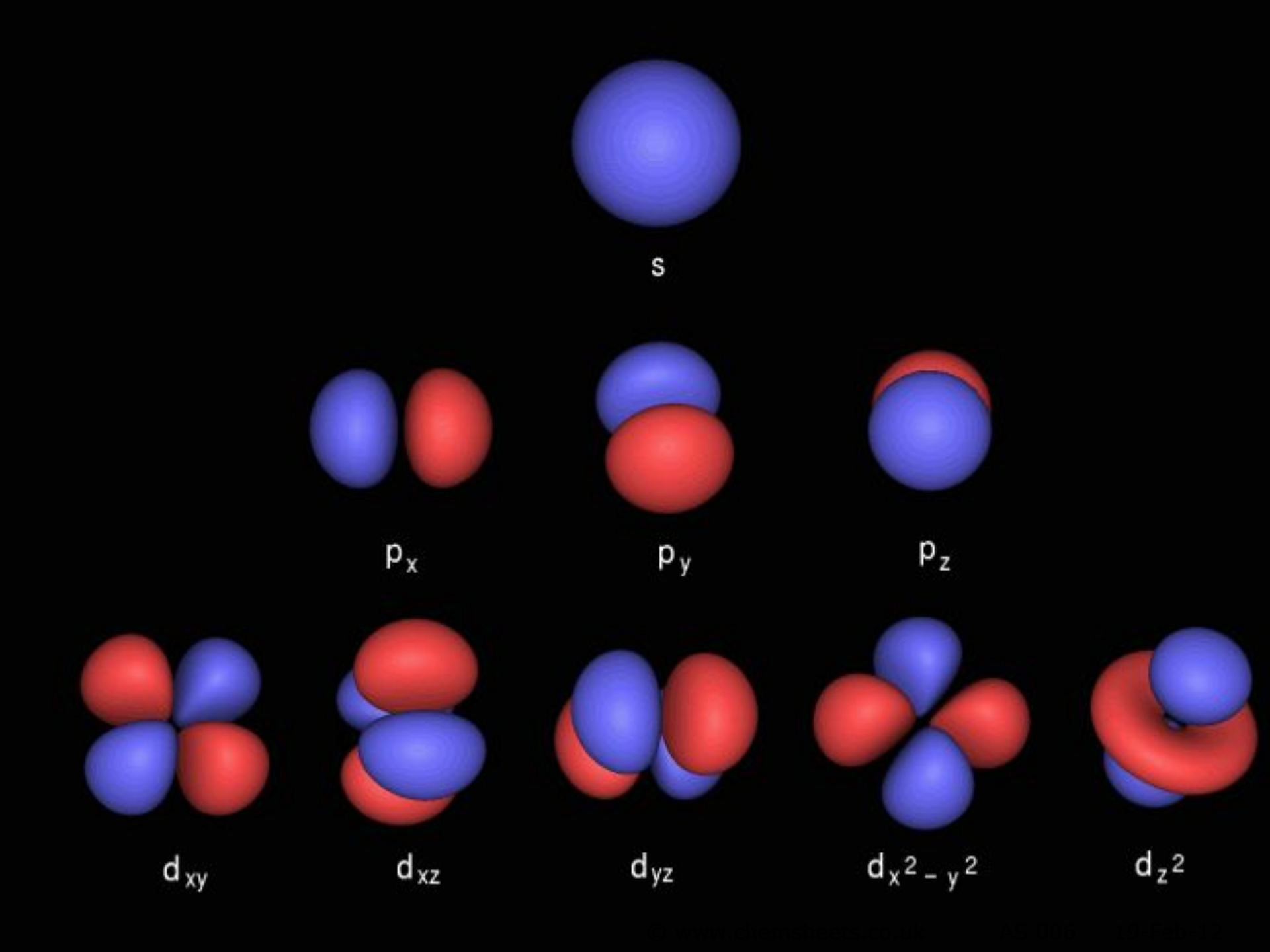
- Each sub-level consists of electron orbitals (region of space in which the electron spends most of its time).
- Each orbital can hold 2 electrons with opposite spins (one electron spins clockwise and one anticlockwise).
- Orbitals are regions of space that electrons are most likely to be in.

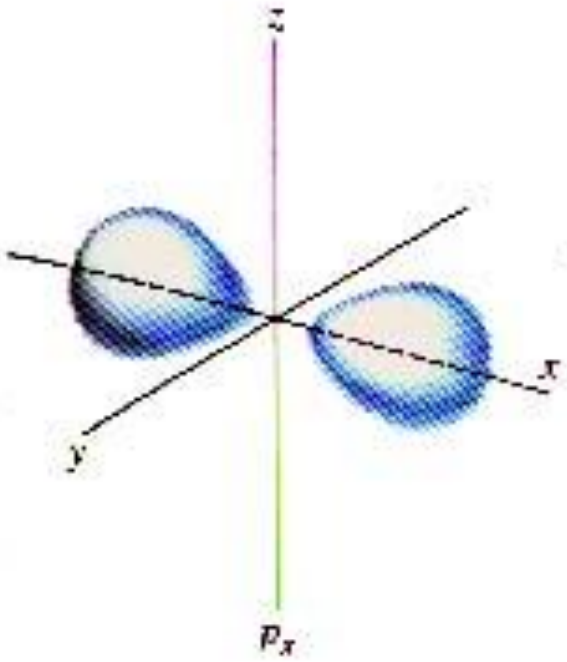


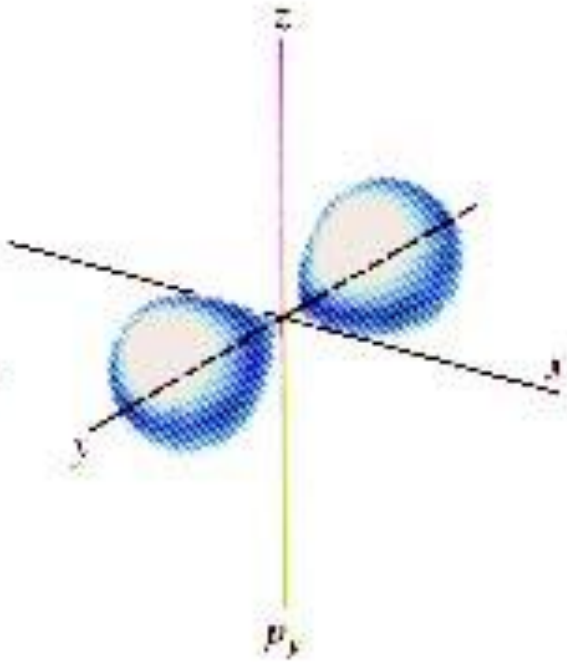
s orbital

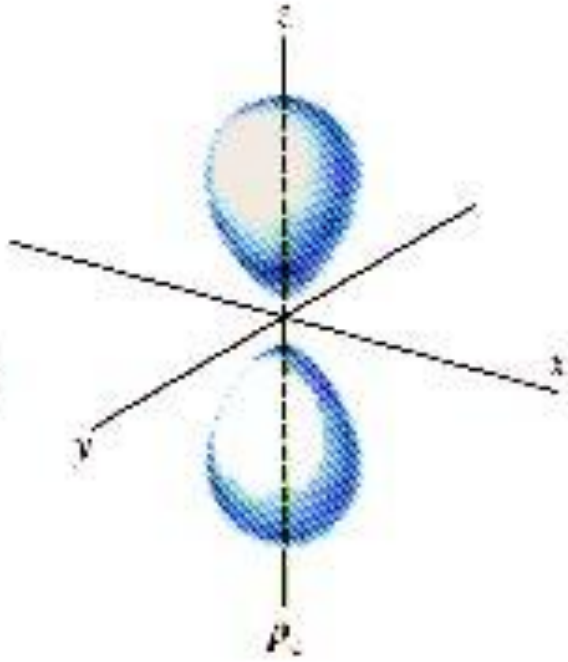


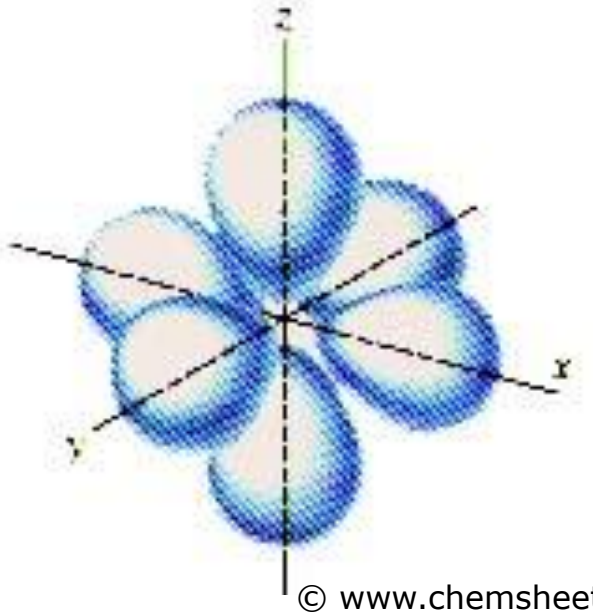
p orbital


s
p_x
p_y
p_z
d_{xy}
d_{xz}
d_{yz}
$d_{x^2-y^2}$
d_{z^2}


z
x
y
p_x

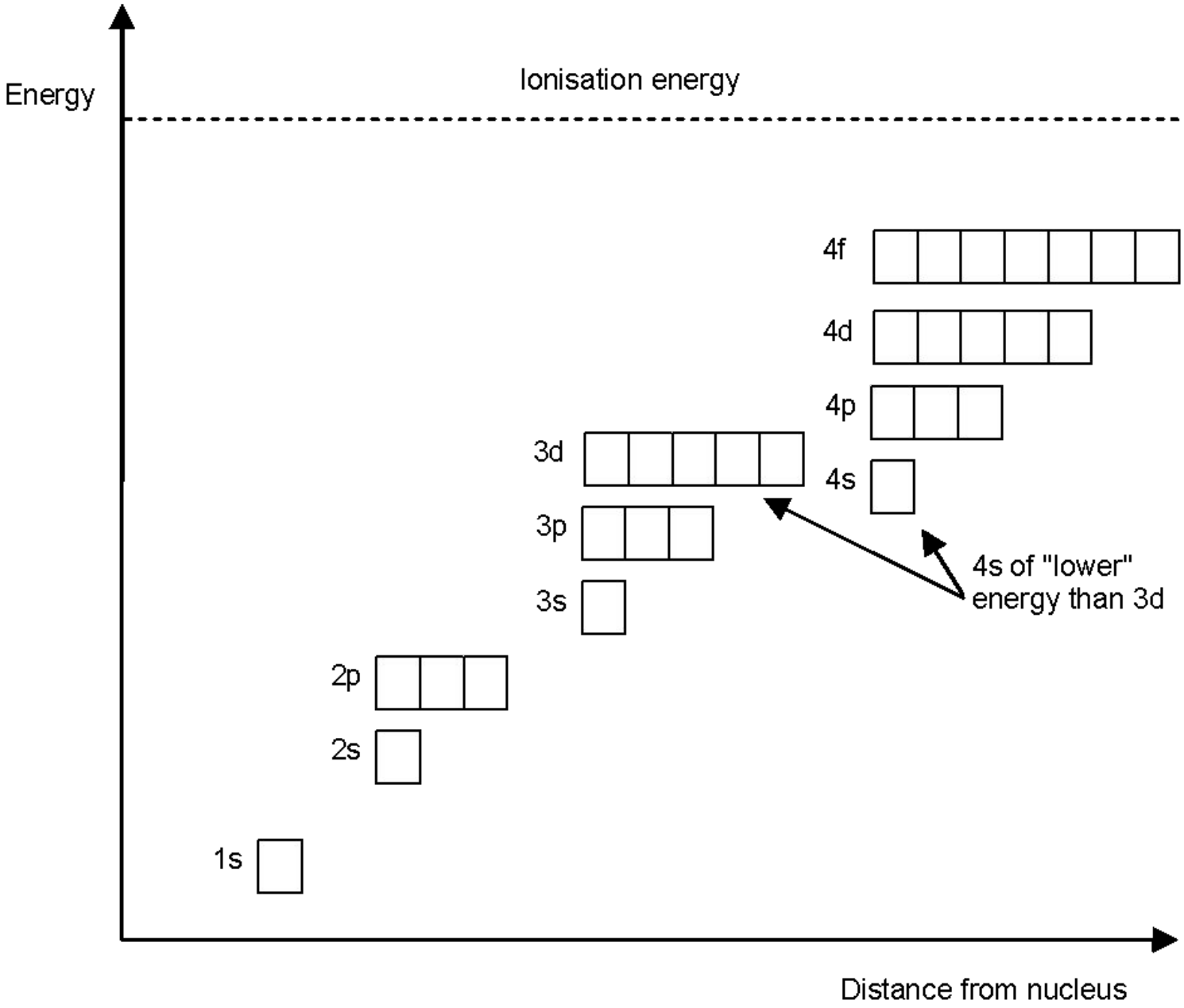

z
x
y
p_y


z
x
y
p_z

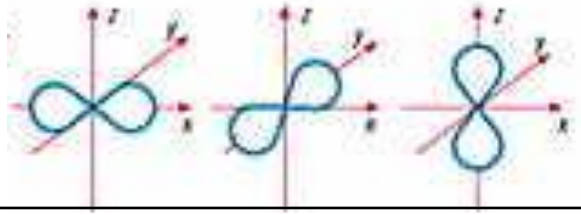
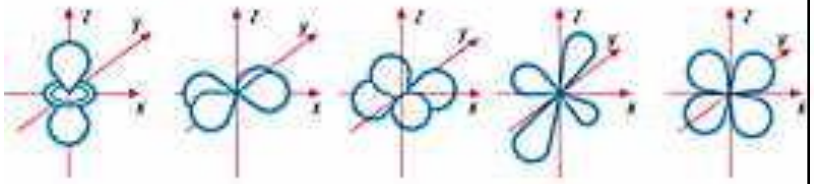

z
x
y

The Orbitron

http://winter.group.shef.ac.uk/orbitron/AOs/1s/index.html


Energy
Ionisation energy
4f
4d
4p
3d
4s
3p
3s
4s of "lower" energy than 3d
2p
2s
1s
Distance from nucleus

Orbitals

Sub-level	Number of orbitals in sub-level	Shape (no need to learn)	Maximum number of electrons in sub-level
s	1		2
p	3		6
d	5		10
f	7	Even more complicated!	14

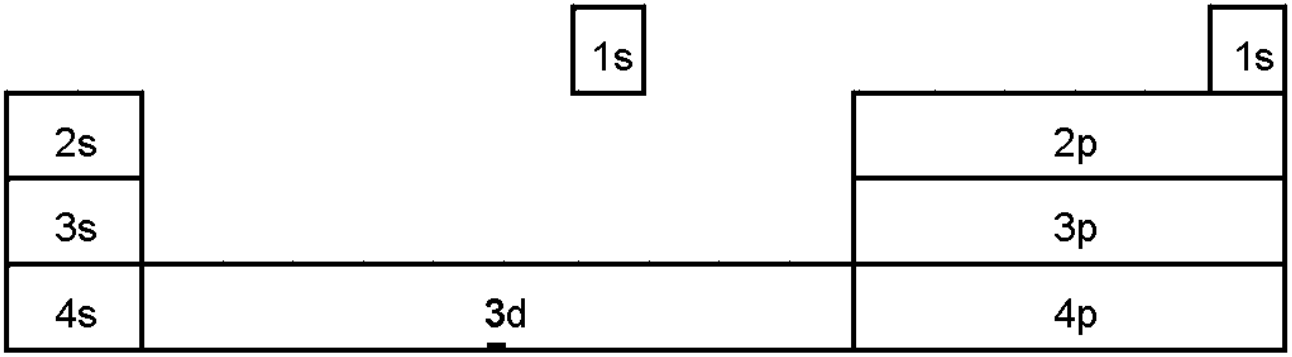
other T-shirts
are available!!

Aufbau Principle

Electrons enter the lowest energy orbital available.

This diagram helps you to work out the order in which orbitals fill:
1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, …..

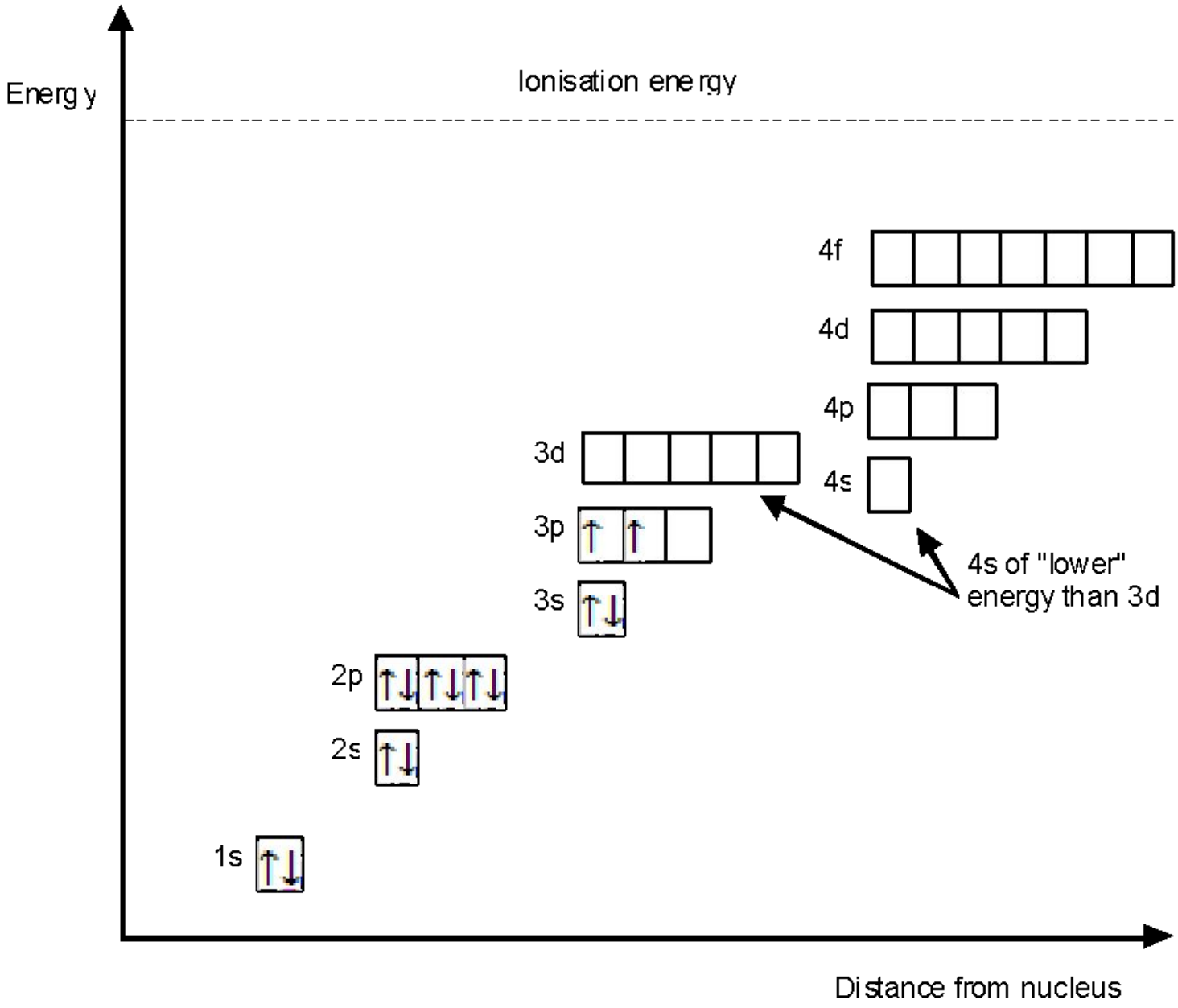
However, it can be easier to read across the periodic table, but remember that the first transition metal row is 3d:



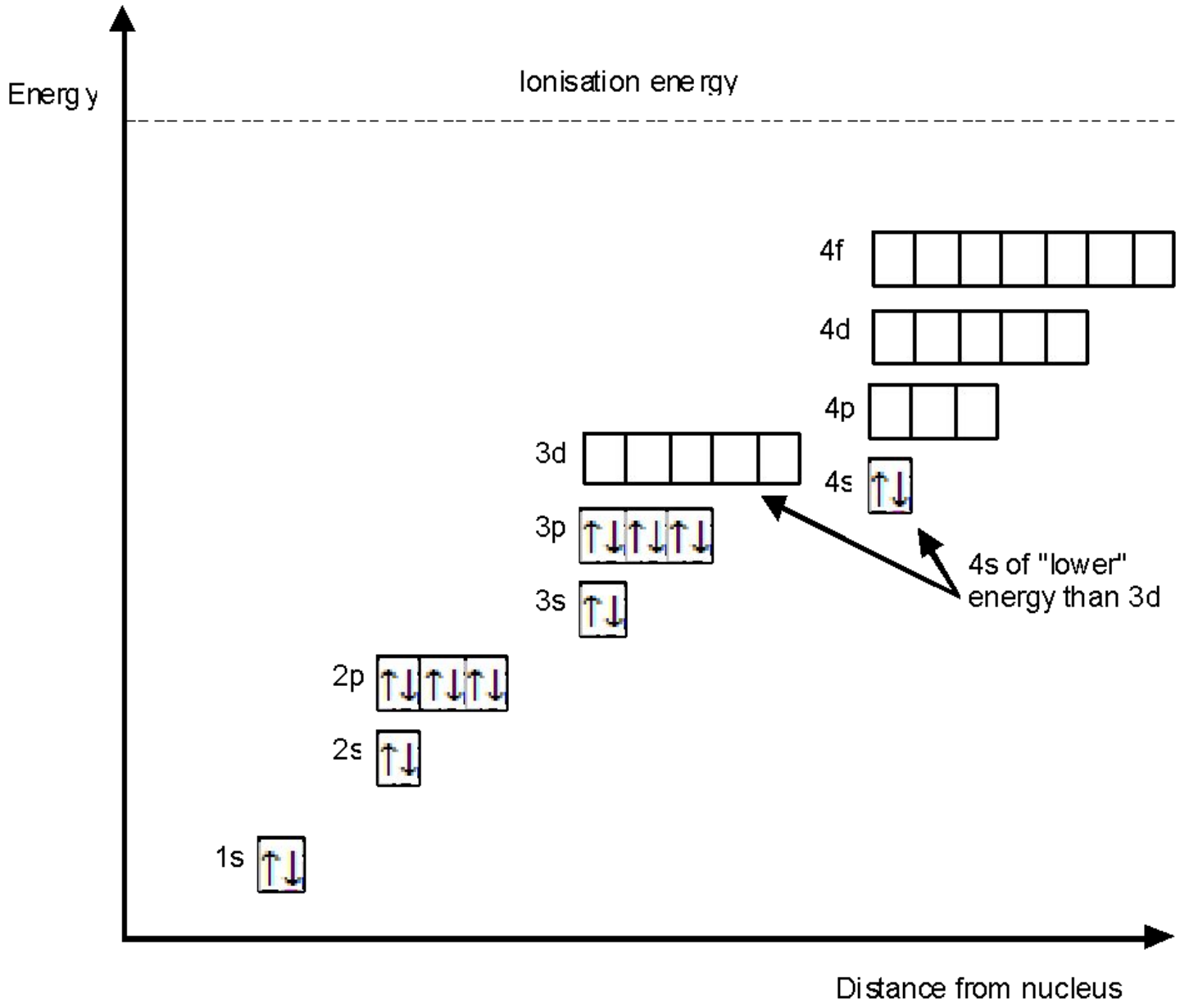
Hund's Rule

Electrons prefer to occupy orbitals on their own, and only pair up when no empty orbitals of the same energy are available .

e.g. silicon 14 e^- $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$



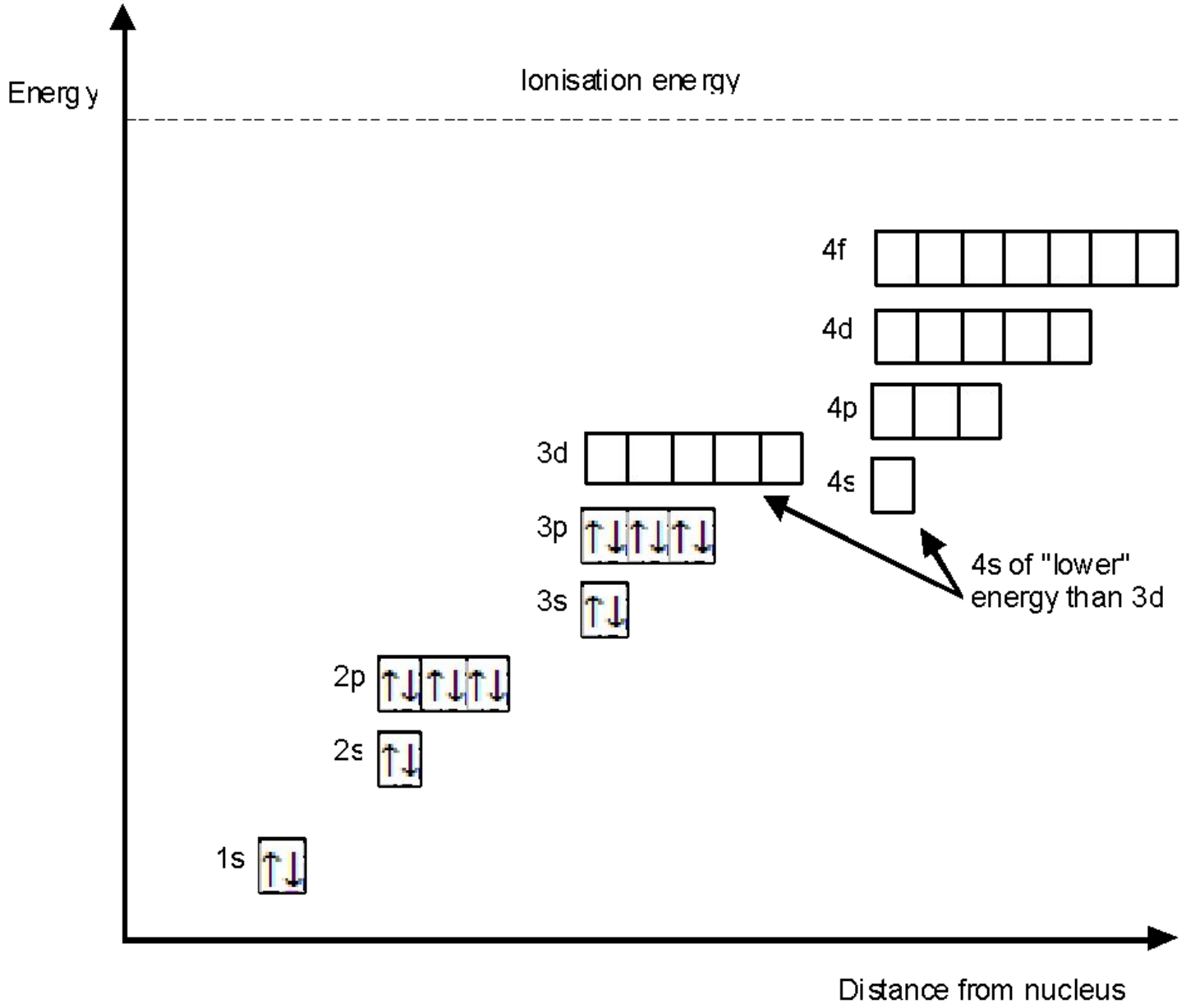
e.g. calcium 20 e^- $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$



Ions

- The highest energy electrons are lost when an ion is formed.
- Note that 4s electrons are lost before 3d (as once 4s and 3d are occupied, 4s moves above 3d).

e.g. Ca^{2+} 18 e^- $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$



Cu & Cr

- Cu and Cr do not have the expected electron structure.

Cr = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 3d^5$
NOT $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^4$

Cu = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 3d^{10}$
NOT $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^9$

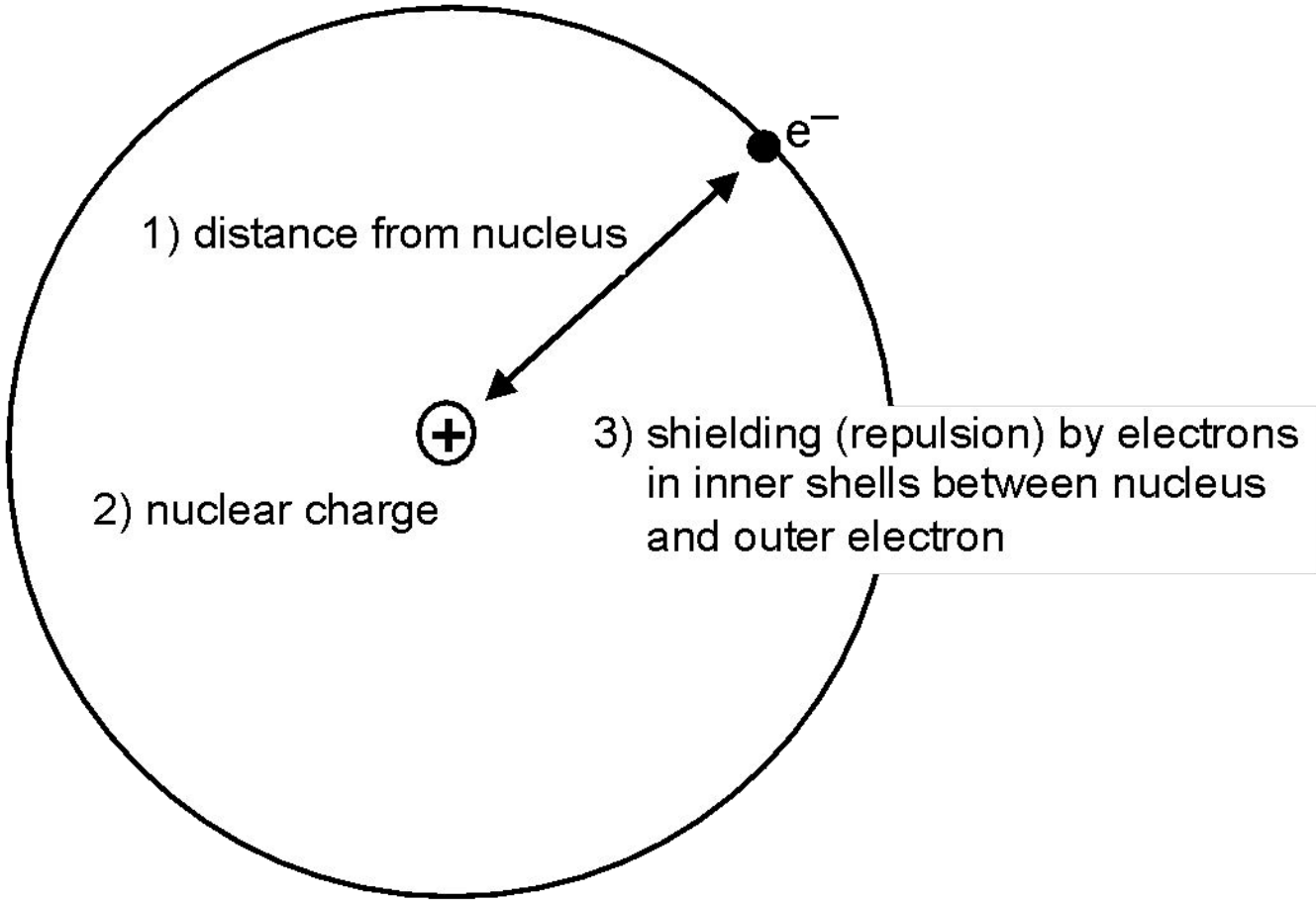
Ionisation Energy

- Evidence for how the electrons are arranged in atoms comes from ionisation energies.
- 1st ionisation energy = energy required to remove one electron from each atom in a mole of gaseous atoms producing one mole of 1+ gaseous ions.
- Note that 2nd ionisation energy is the energy required to remove the second electron (not both electrons).

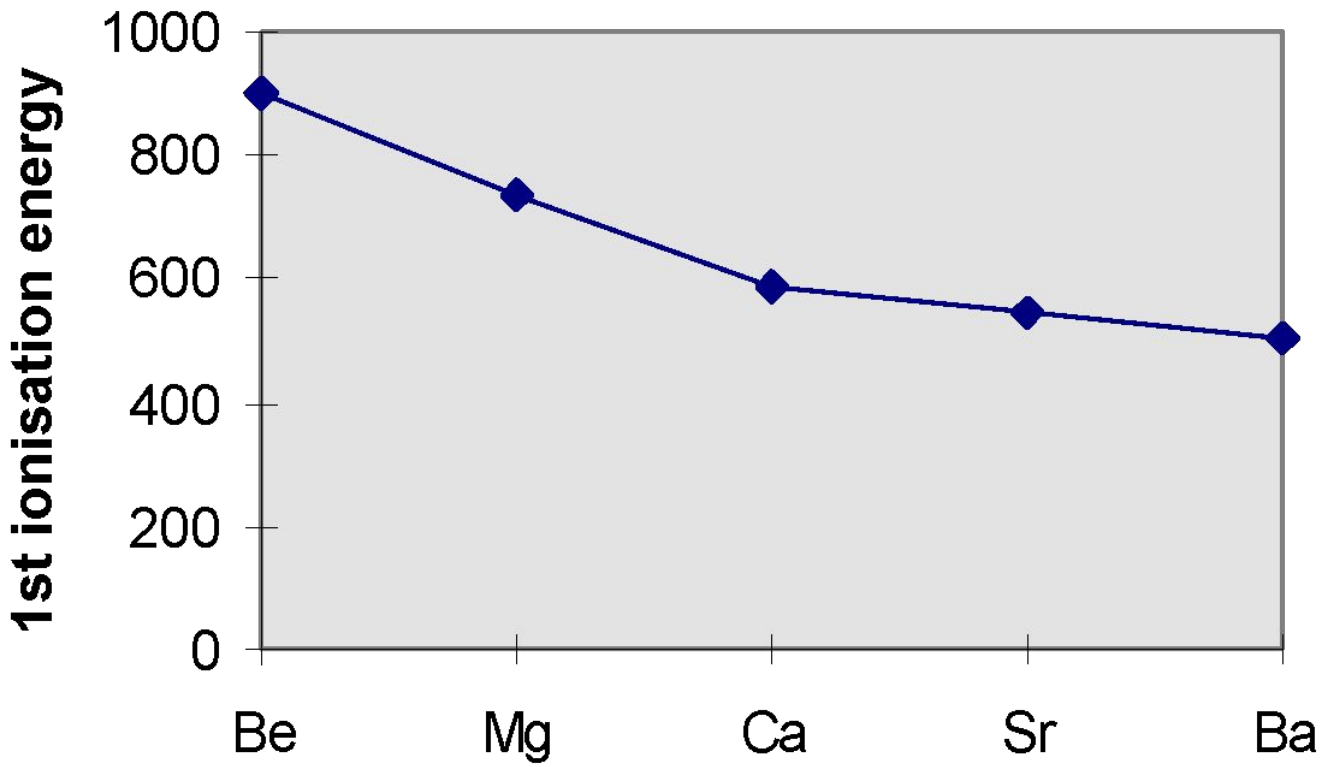
e.g. 1st IE of Na: $Na(g) \rightarrow Na^{+}(g) + e^{-}$

2nd IE of Na: $Na^{+}(g) \rightarrow Na^{2+}(g) + e$

Ionisation Energy



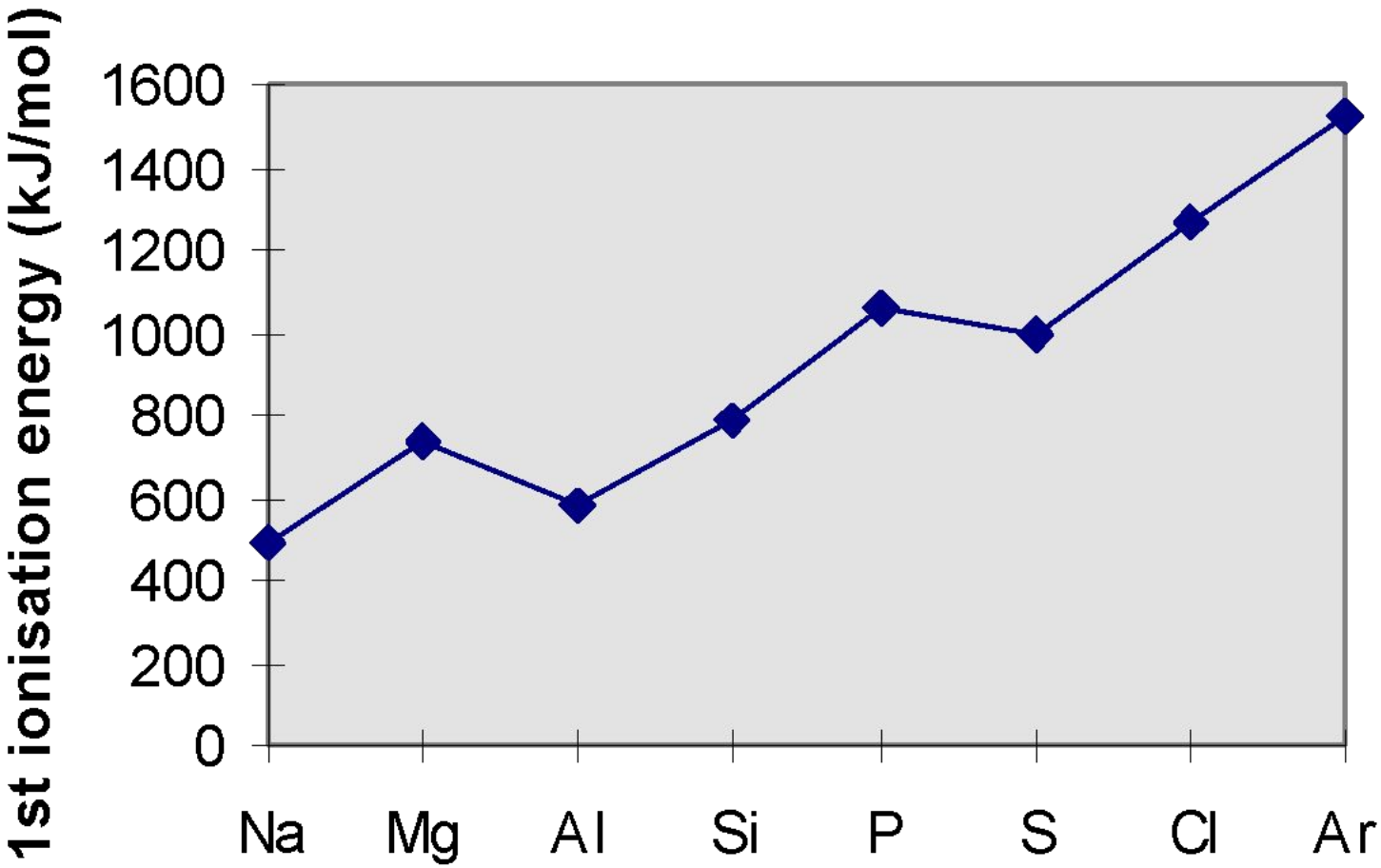
1st ionisation energy (down group)



1st ionisation energy (down group)

- Atoms get bigger
- More shielding
- Therefore weaker attraction from nucleus to electron in outer shell

1st ionisation energy (across period)



1st ionisation energy (across period)

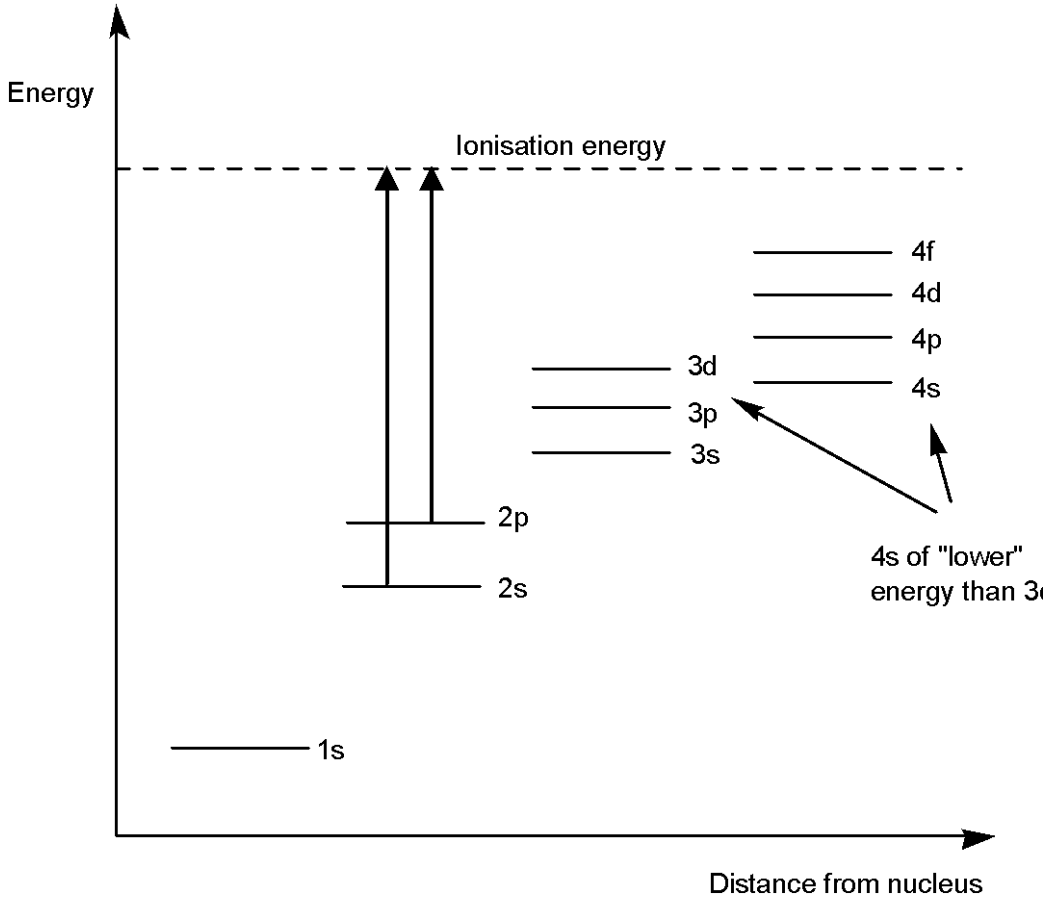
General trend

- Increased nuclear charge (i.e. more protons)
- Atoms get smaller
- Therefore stronger attraction from nucleus to electron in outer shell

1st ionisation energy (across period)

Group 2 → 3

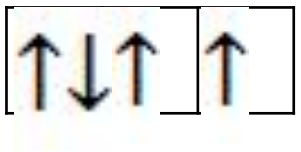
- Electron lost from Group 3 element is from p orbital, while that lost from Group 2 element is from s orbital.
- p orbital is higher energy than s orbital, so easier to lose electron.



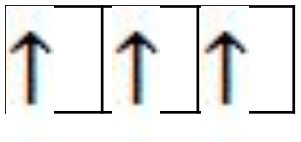
1st ionisation energy (across period)

Group 5 → 6

- Group 6 element loses electron from orbital with 2 electrons (p^4)

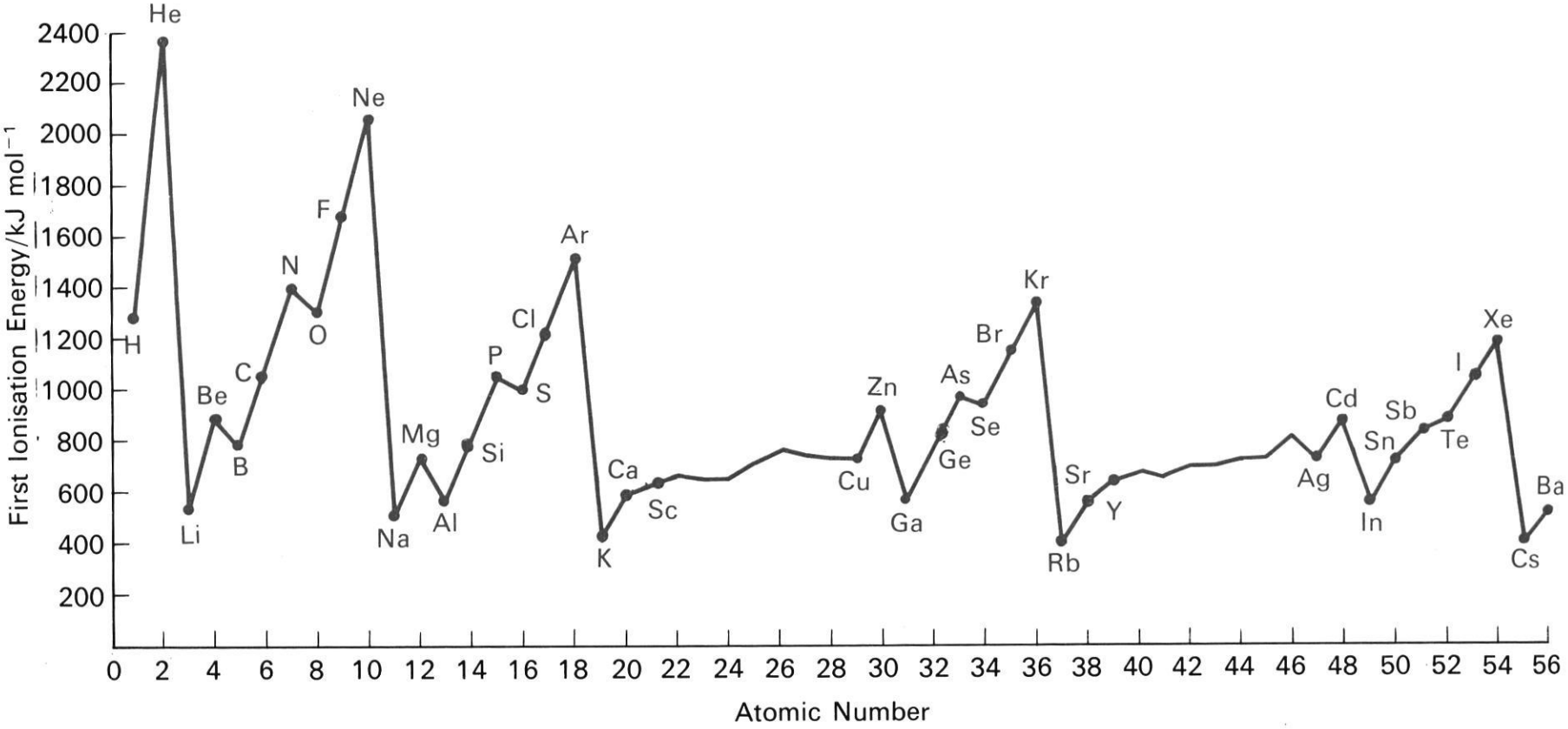


- Group 5 element loses electron from orbital with 1 electrons (p^3)



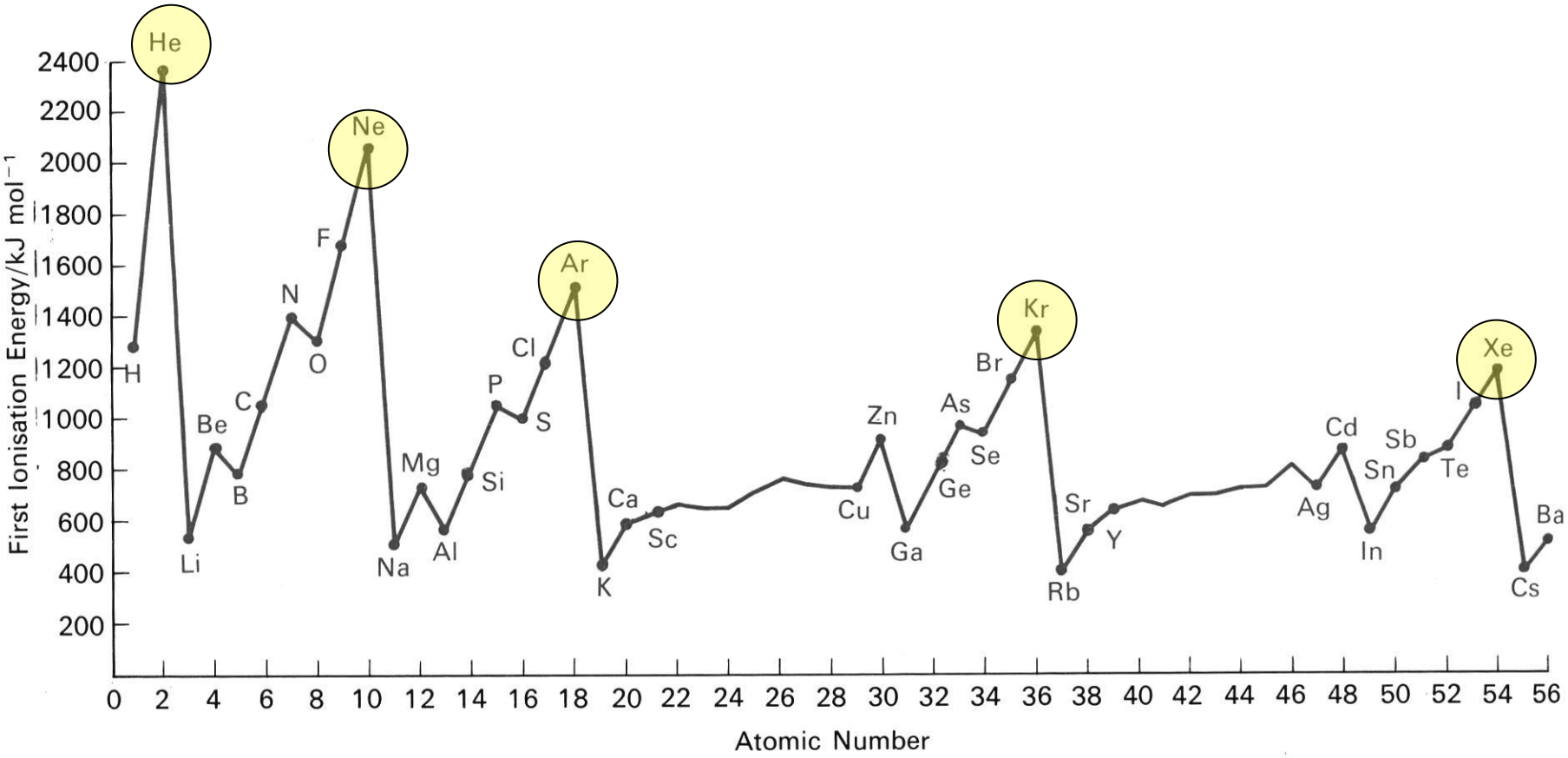
- Extra electron-electron repulsions make it easier to lose electron from p^4 than p^3.

1st ionisation energy



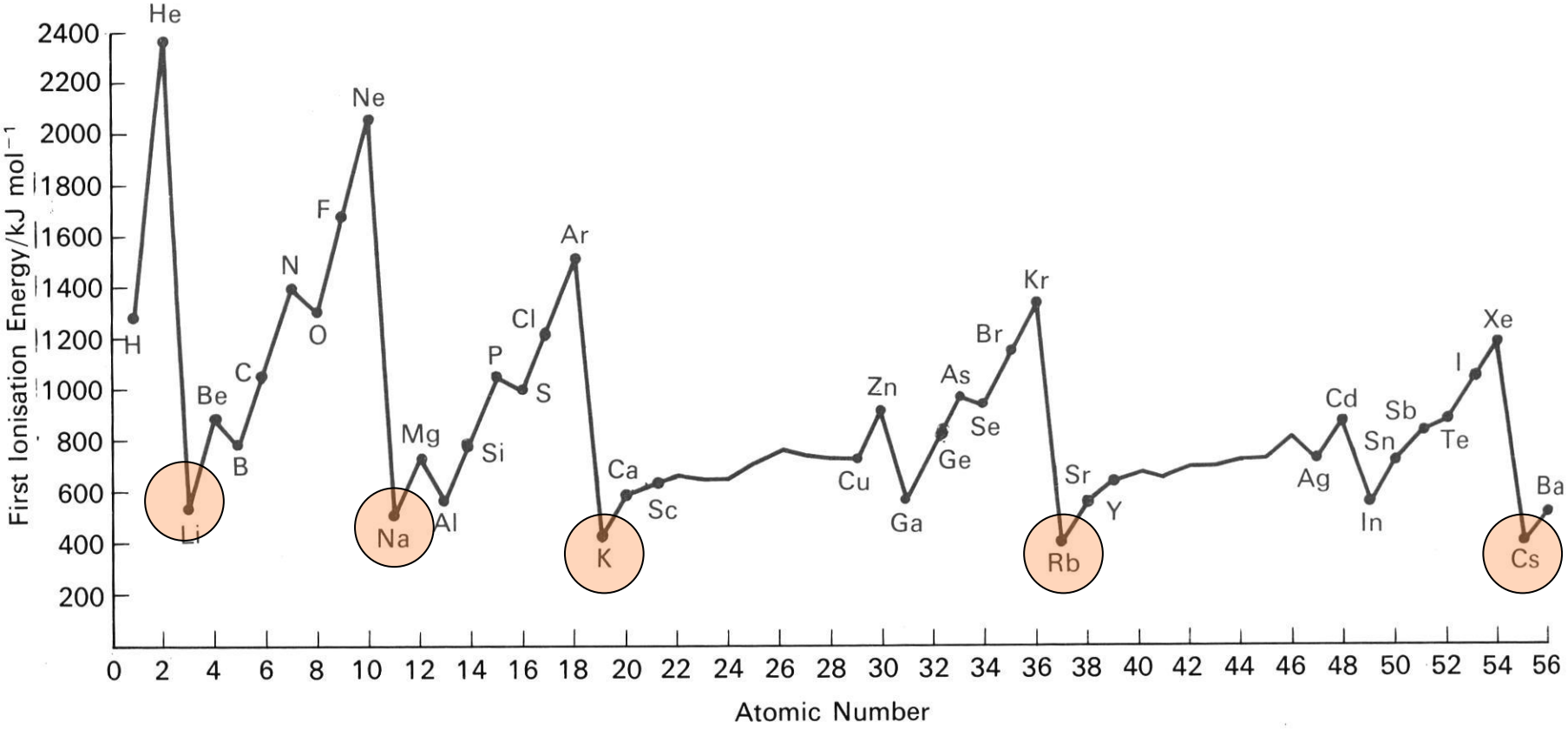
down a group (group 0)

1st ionisation energy



down a group (group 1)

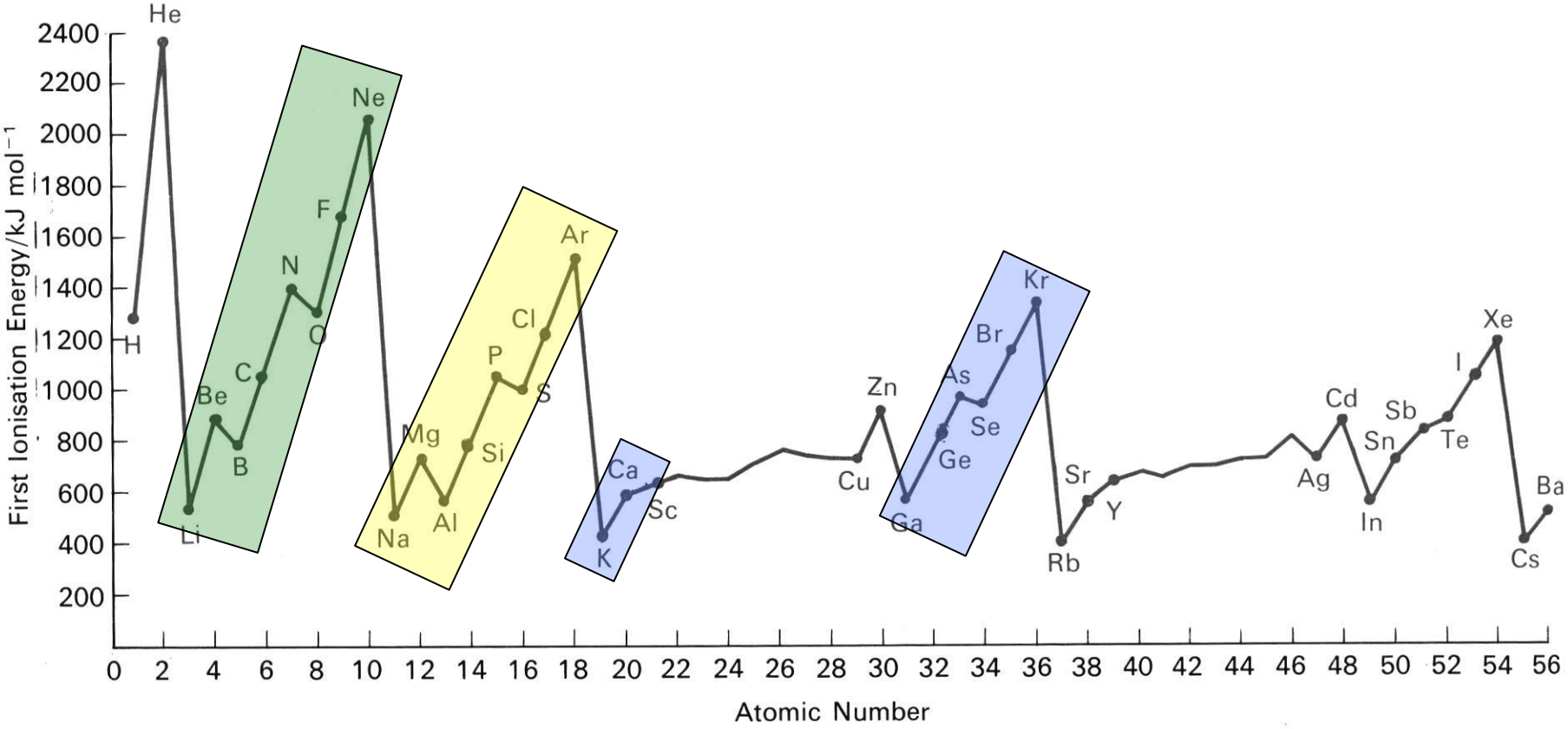
1st ionisation energy



Across a period

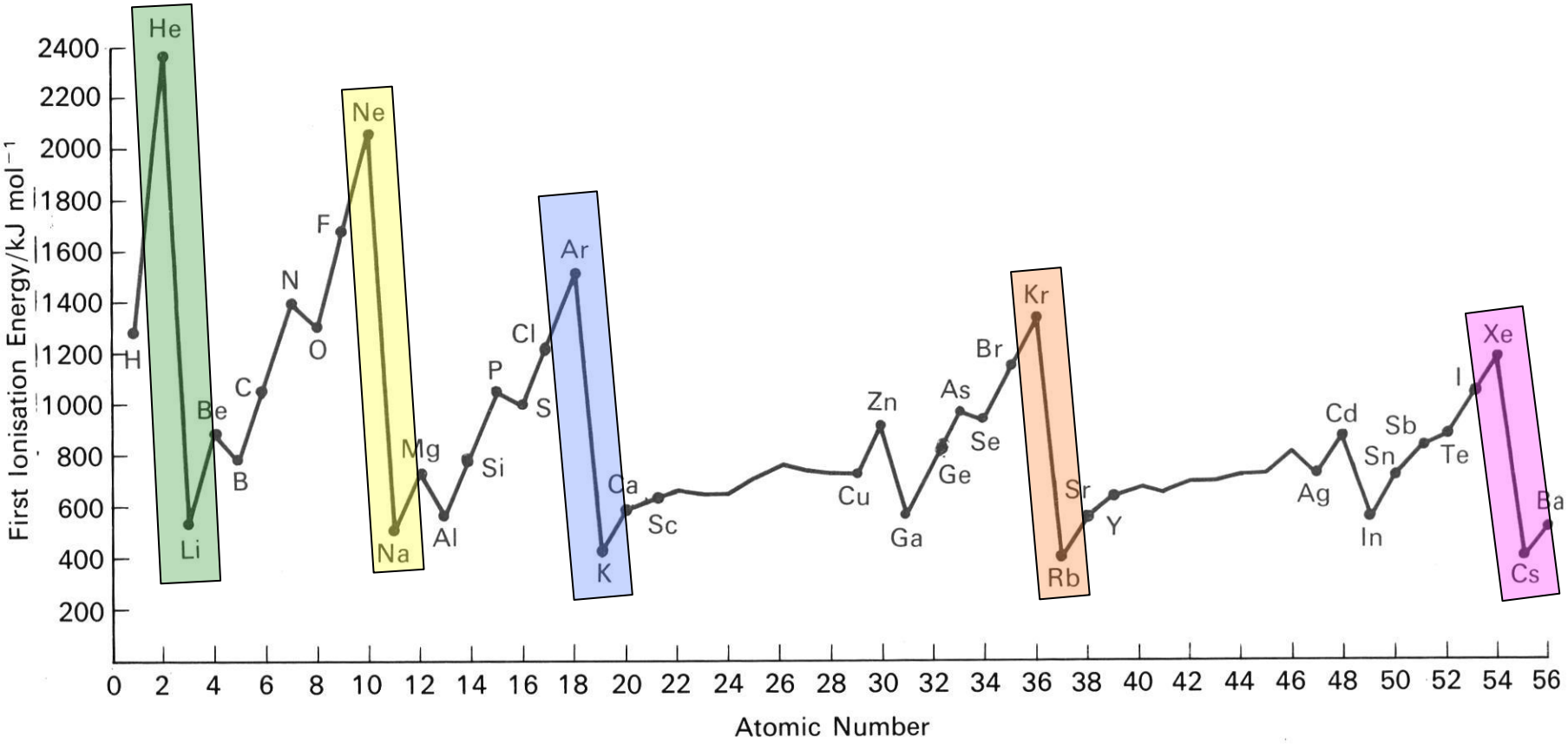
period 2
period 3
period 4

1st ionisation energy



End of period

1st ionisation energy



Successive ionisation energies (K)