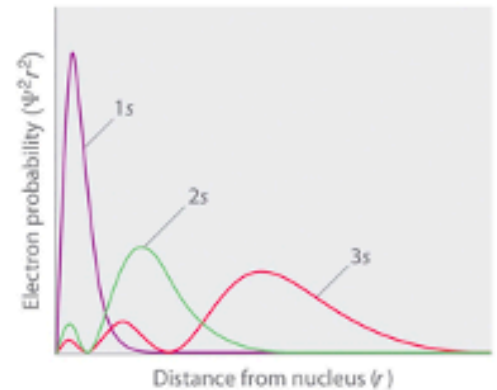


## Quantum Numbers

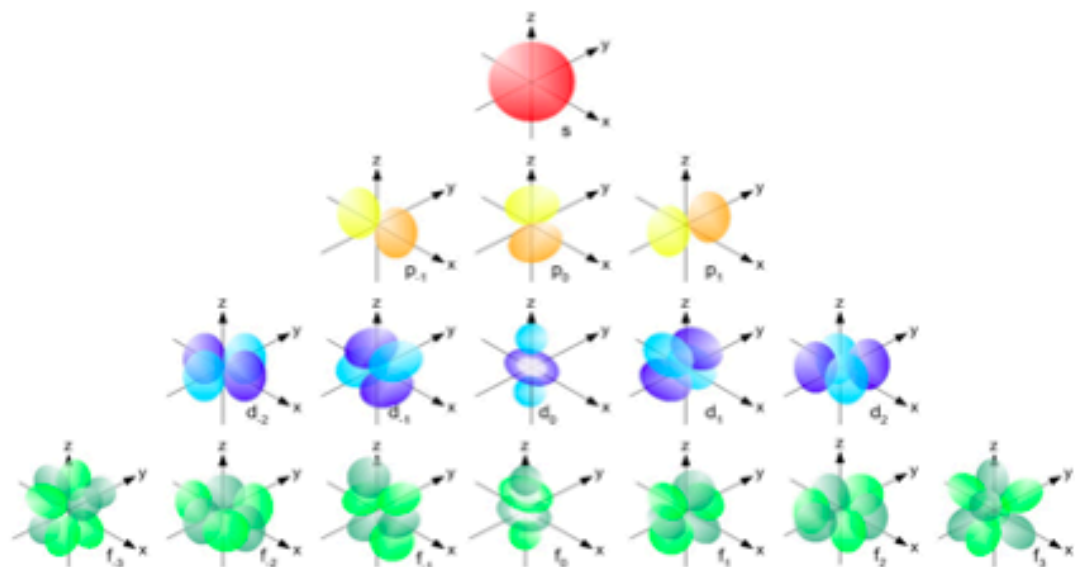
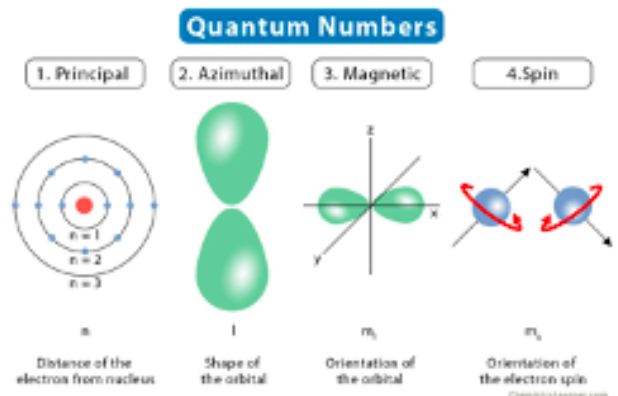
- Describe the quantum state of electrons (there are 4 numbers:)

- o Principal quantum number ( $n$ ): Determines size and energy of orbital (e.g.  $n=1,2,3\dots$ ). Energy and distance from nucleus increase with  $n$ 
  - In between orbitals (of varying  $n$ ) are nodes, which follows from the quantisation of orbital energies
  - Graphing square of wave function vs. distance from the nucleus gives the graph to the right, showing the peak probabilities in each orbital occur at different distances for each ' $n$ '



- o Angular quantum number ( $\ell$ ): Determines shape of the orbital, denoted by s, p, d and f orbitals ( $\ell = 0, 1, 2, \dots (n-1)$ )
  - $0 = s$
  - $1 = p$
  - $2 = d$
  - $3 = f$

- o Magnetic quantum number ( $m_\ell$ ): Denotes the orientation of the orbital (on which axis it lies)
  - As seen above,  $m_\ell$  ranges from  $-\ell$  to  $+\ell$
- o Spin quantum number ( $m_s$ ): Denotes spin of electron (either  $+1/2$  or  $-1/2$ )



## Pauli Exclusion Principle

- No two electrons in the same atom can have the same set of four quantum numbers and no orbital can contain more than two electrons (this occurs because every electron occupies different orbitals, and two electrons in the same orbital have opposite spin numbers)
  - o Limited number of electrons in each orbital to 2 (with opposite spin)
- In Hydrogen the energy of the sub-shells of a given n are degenerate (of the same energy)
- In all other atoms the sub-shells are of different energies

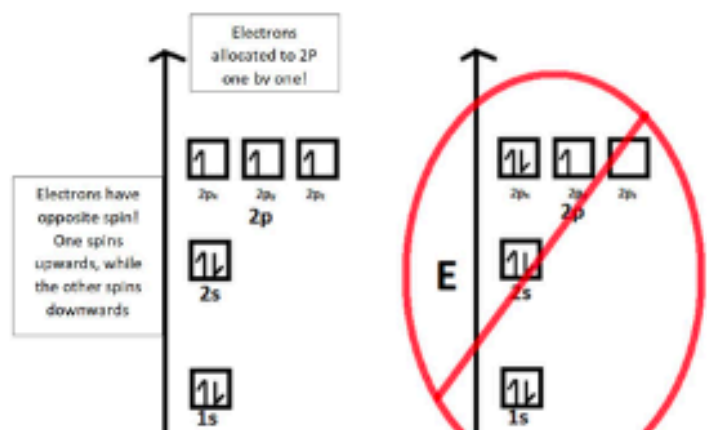
Rules to follow:

- o **Aufbau Principle:** Electrons occupy orbitals in increasing energy (1 → 3...)
- o **Madelung's rule:** orbitals fill according to this diagram → → →

|     | $l=0$  | $l=1$  | $l=2$     | $l=3$     |     |
|-----|--------|--------|-----------|-----------|-----|
| n=1 | $1s^2$ |        |           |           | 2 → |
| n=2 | $2s^2$ | $2p^6$ |           |           |     |
| n=3 | $3s^2$ | $3p^6$ | $3d^{10}$ |           |     |
| n=4 | $4s^2$ | $4p^6$ | $4d^{10}$ | $4f^{14}$ |     |
| n=5 | $5s^2$ | $5p^6$ | $5d^{10}$ | $5f^{14}$ |     |
| n=6 | $6s^2$ | $6p^6$ | $6d^{10}$ | $6f^{14}$ |     |
| n=7 | $7s^2$ | $7p^6$ | $7d^{10}$ | $7f^{14}$ |     |

- S subshell = 2 electrons
- P subshell = 6 electron
- D subshell = 10 electrons
- F subshell = 14 electrons
- Notation can be shortened used [Noble gas name] + config after the noble gas (e.g. [Ar]  $4s^1$ )

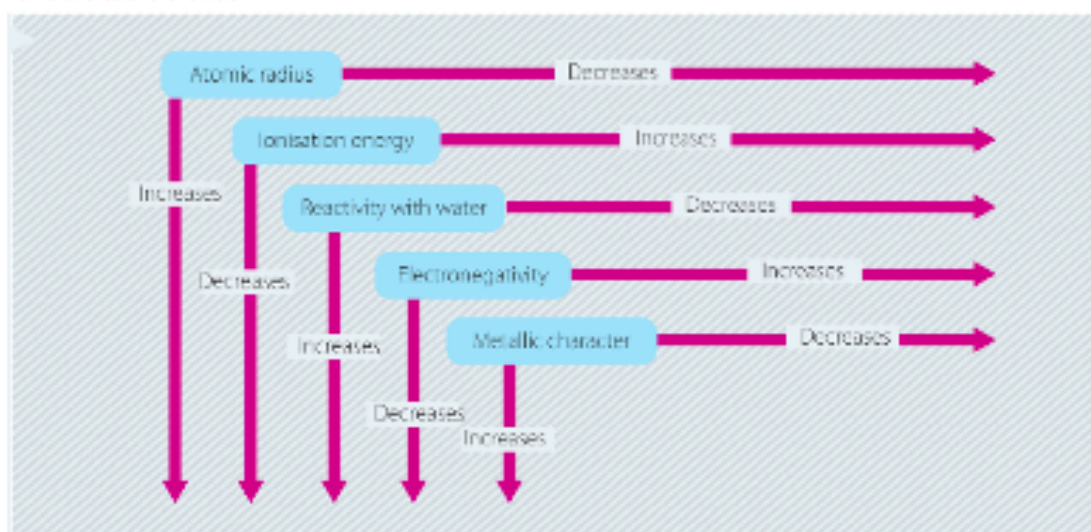
- o **Hund's Rule:** When electrons occupy orbitals with the same energy, they must first occupy the empty orbitals before double occupying them.
- o **Pauli-Exclusion Principle:** Electrons in the same orbital must have opposite spins.



Excited state of Na:  $1s^2 2s^2 2p^6 3s^1 \rightarrow 1s^2 2s^2 2p^6 3s^0 3p^1$

- When electron returns to ground state, yellow light is emitted

Periodic table trends



Nuclear Charge ( $Z$ ) = Number of protons in nucleus

Effective nuclear charge ( $Z_{\text{eff}}$ ) = positive charge felt by n electron in a multi-electron atom

- $Z_{\text{eff}}$  decreases as more electrons orbit closer to the nucleus (shielding effect)
- Electrons further from the nucleus experience a lower  $Z_{\text{eff}}$
- Atomic radius decreases across a period and increases down a group
  - o Trend reflects effective nuclear charge
  - o This is because more protons and electrons are added but not in a higher energy level, so the electrostatic attraction is bigger and the radius gets smaller
- Ionic radius = radius of ion
  - o Cation radius < neutral atom (electrons removed, + charge)
  - o Anion radius > neutral atom (electrons added, -ve charge)

First Ionisation Energy: Energy needed to remove one valence electron

- Decreases down a group, increases across a period
- More energy = harder to ionise
- Down a group, a new energy level is added, placing electrons further from the nucleus, meaning they are bonded weakly to the nucleus, making them easier to ionise
- Across a period, more electrons are added to energy levels, meaning they have a stronger bond with the nucleus, making it harder to ionise. Group 8 has a full shell and is stable and also bonded strongly with the nucleus, making it the hardest to ionise.

Electronegativity: Measure of attraction of an atom in a molecule for the electron pair in the covalent bond of which is a part of

- Decreases down a group, increases across a period
- Down a group, electrons are further from the nucleus, allowing them to be removed easier (and shielding effect)
- Across a period, more electrons are added, meaning that >group 14 has the tendency to gain electrons to achieve stability (full orbital configuration), giving them higher electronegativities
- Noble gases are inert and hence have much higher electronegativities