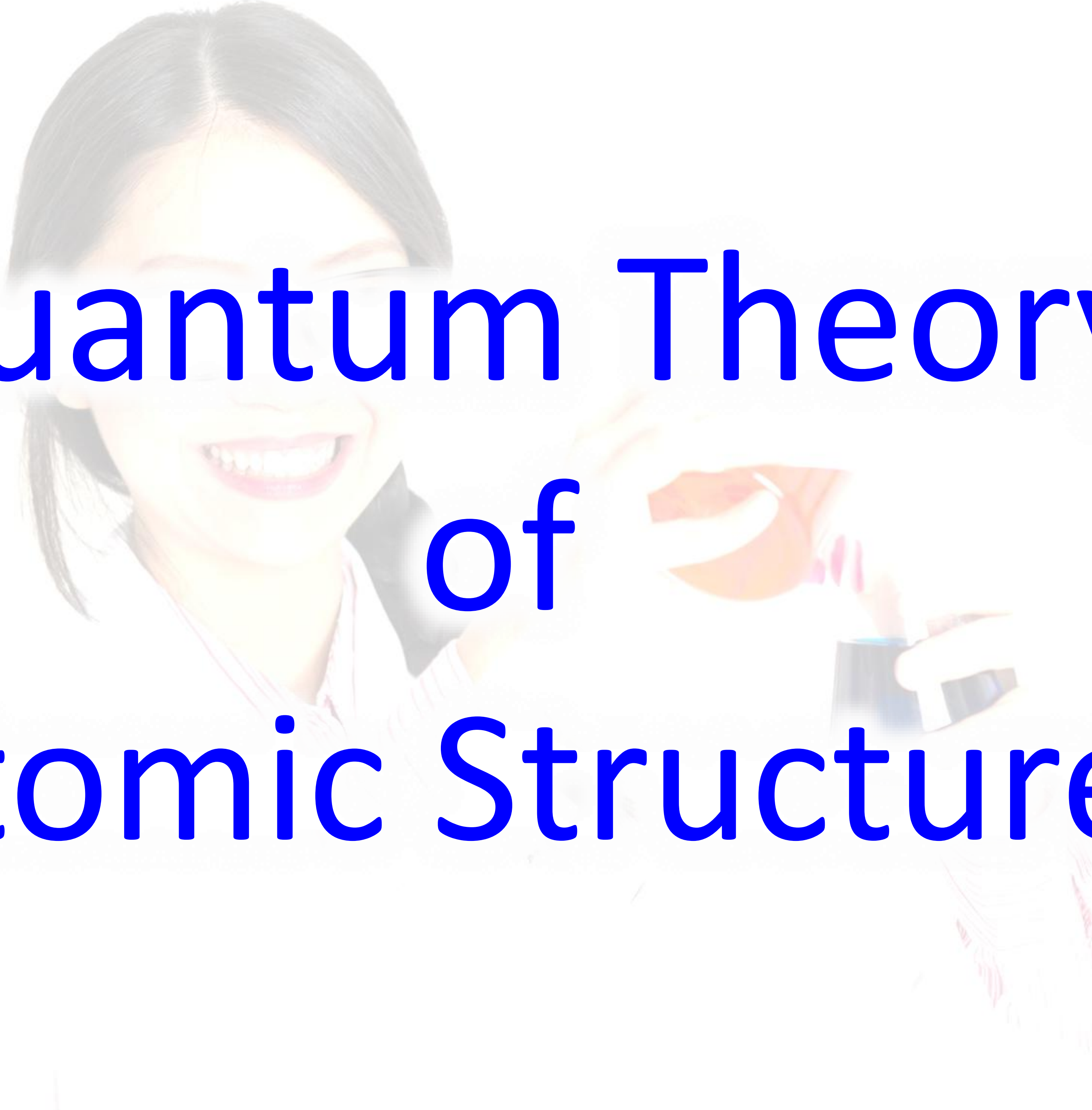
Quantum Theory of Atomic Structure

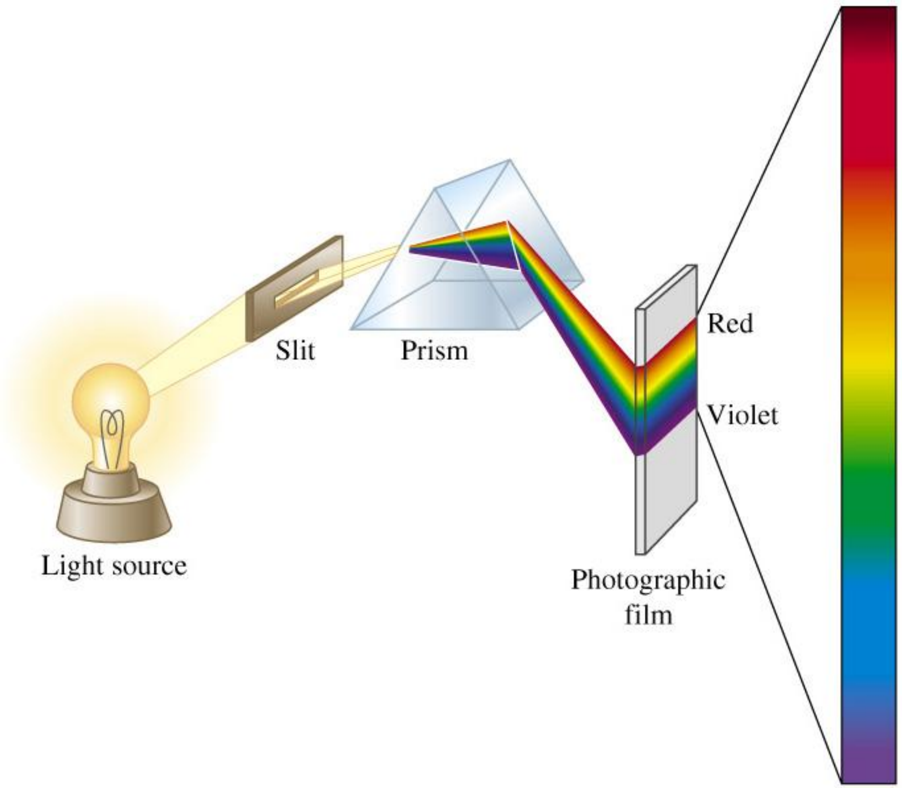


STUDENT ADVISORY

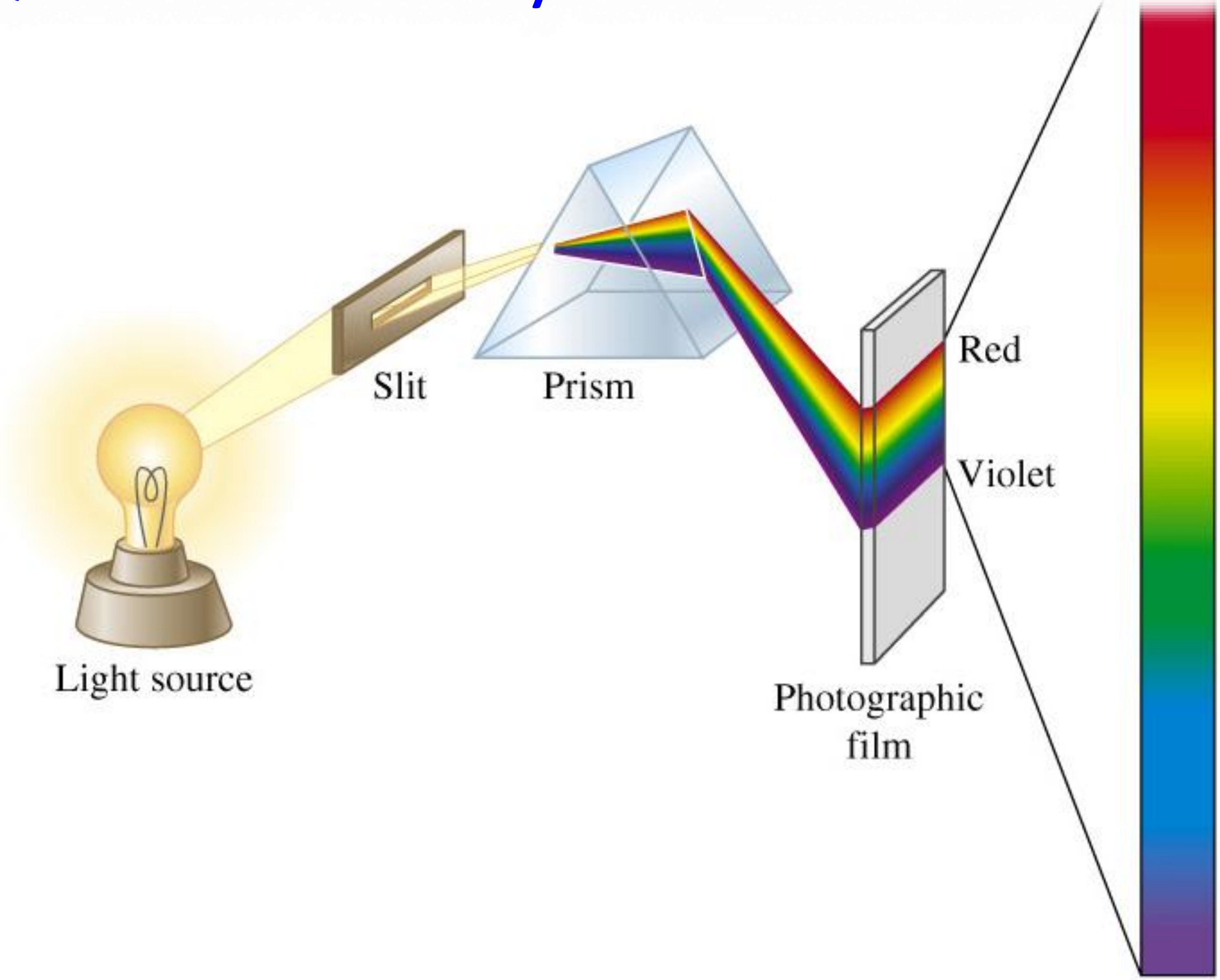
ADVANCED CONCEPTS

Quantum Theory of Atomic Structure

- If white light is shone through a prism, it is *diffracted* to produce a *continuous spectrum* of colours; red, orange, yellow, green, blue, indigo and violet.

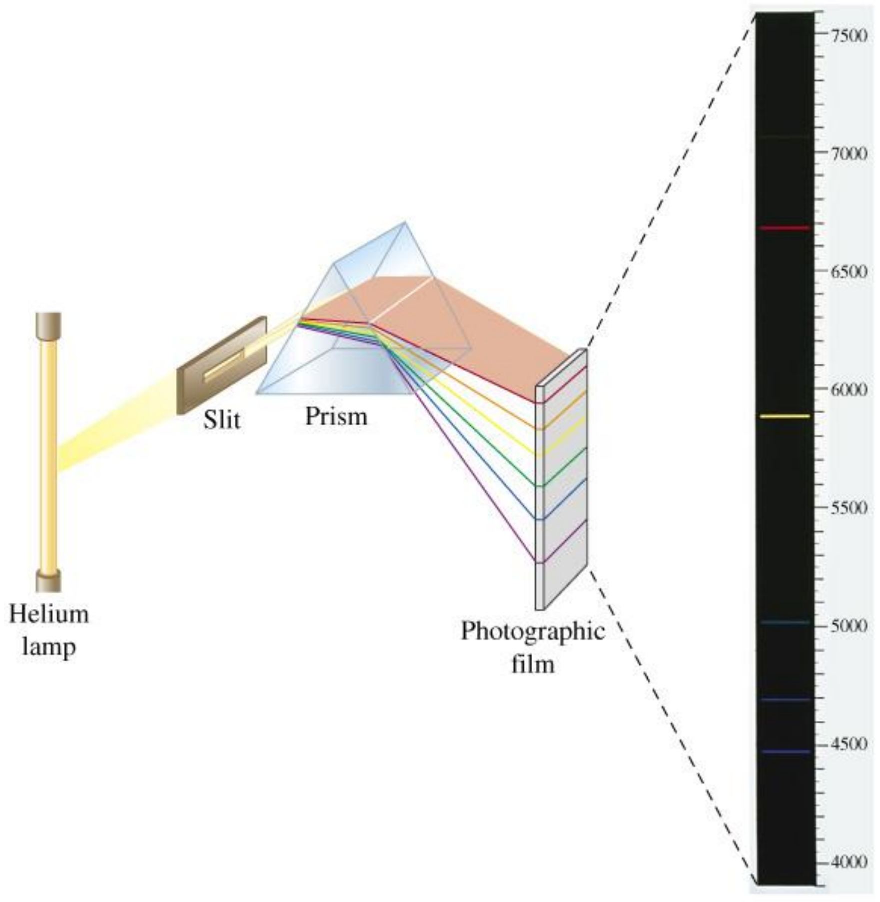


Quantum Theory of Atomic Structure



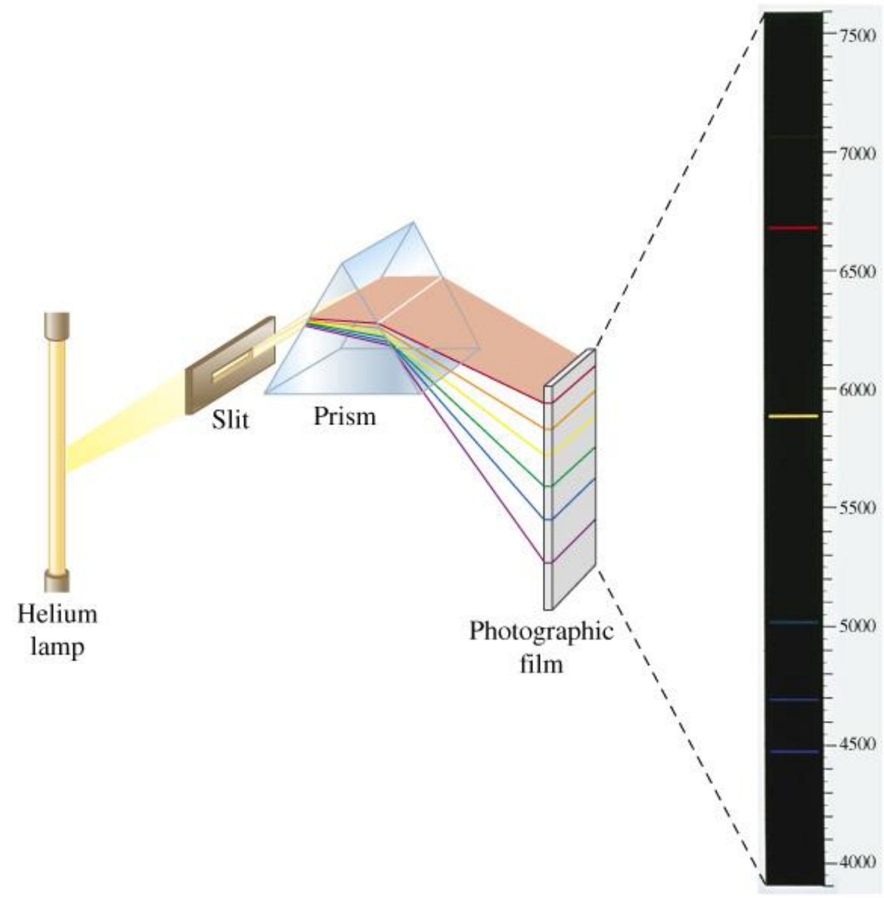
Quantum Theory of Atomic Structure

- If atoms and molecules are heated to sufficiently high temperatures, they emit light of certain wavelengths.



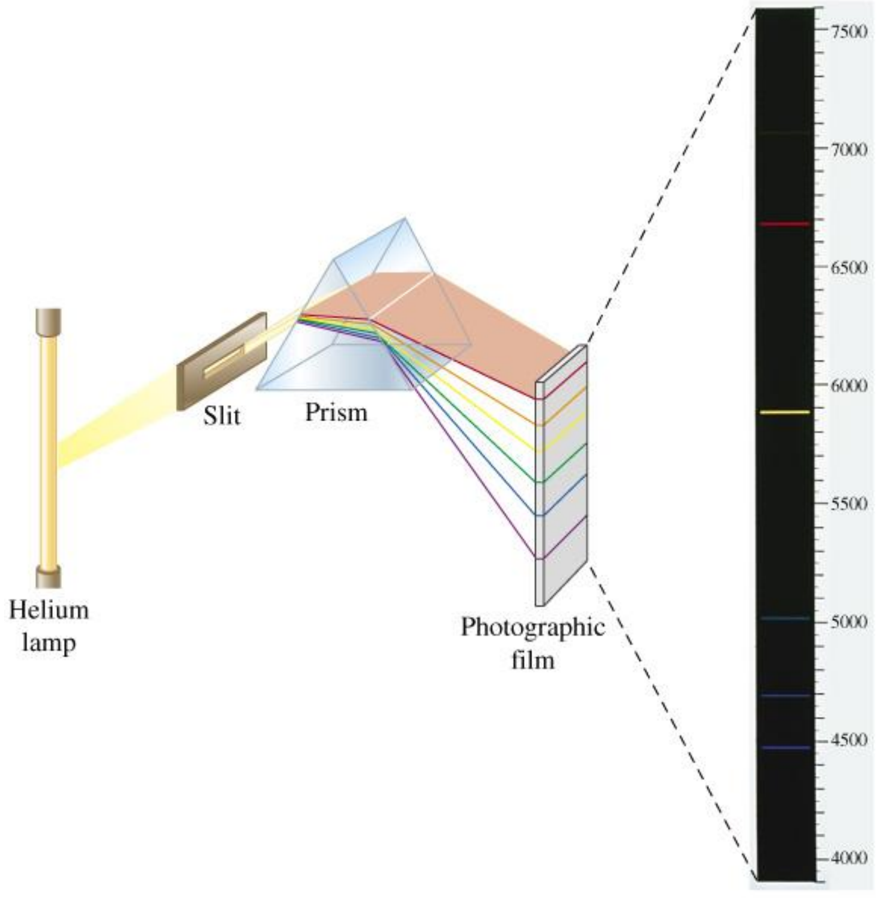
Quantum Theory of Atomic Structure

- The diagram below shows a discharge tube containing a gaseous element. Note the spectrum that is produced is a *discrete spectrum*, not a *continuous spectrum*.

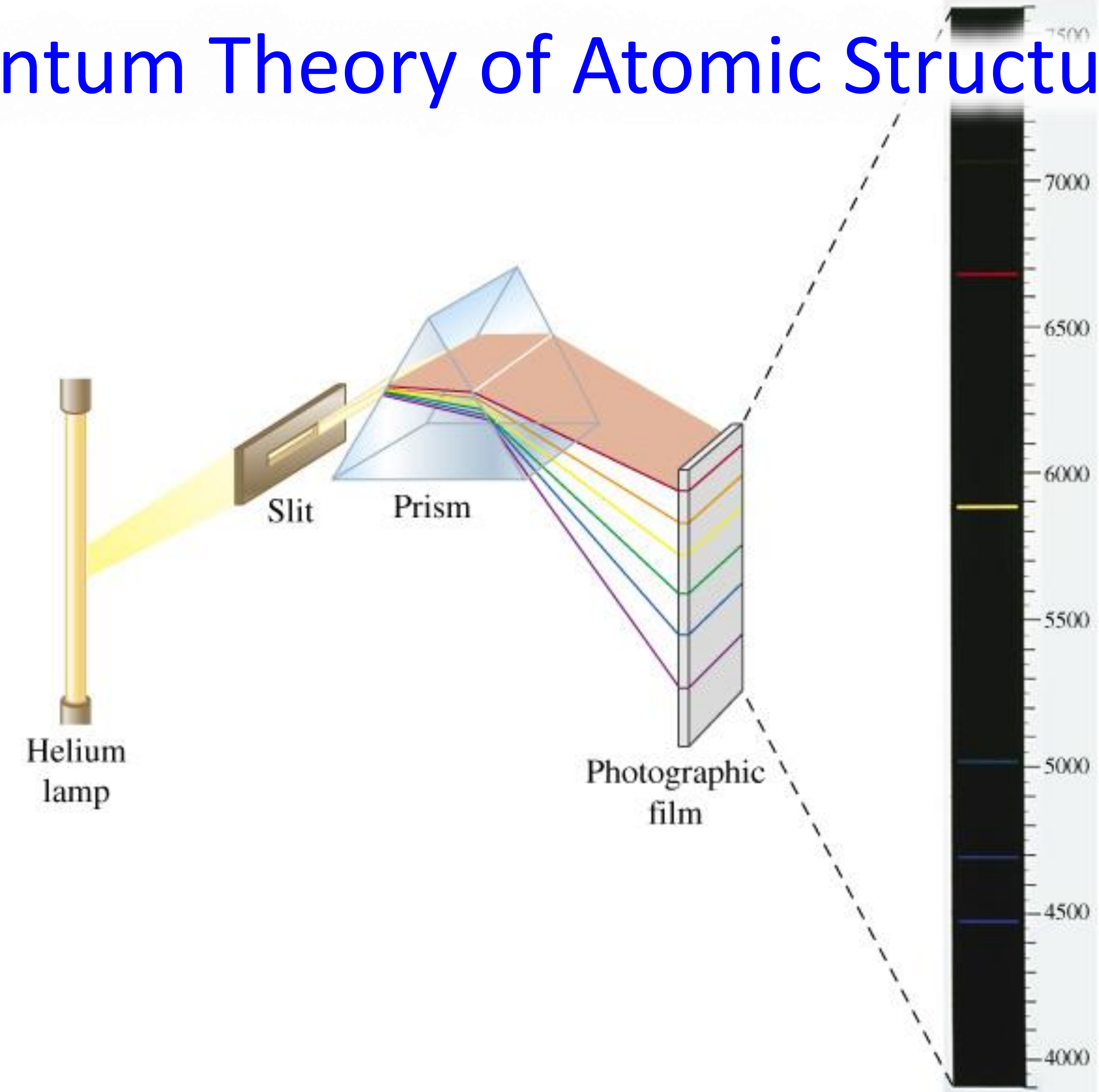


Quantum Theory of Atomic Structure

- The observed spectrum consists of a number of coloured lines on a black background. The spectrum is called an *atomic emission spectrum* or *line spectrum*.

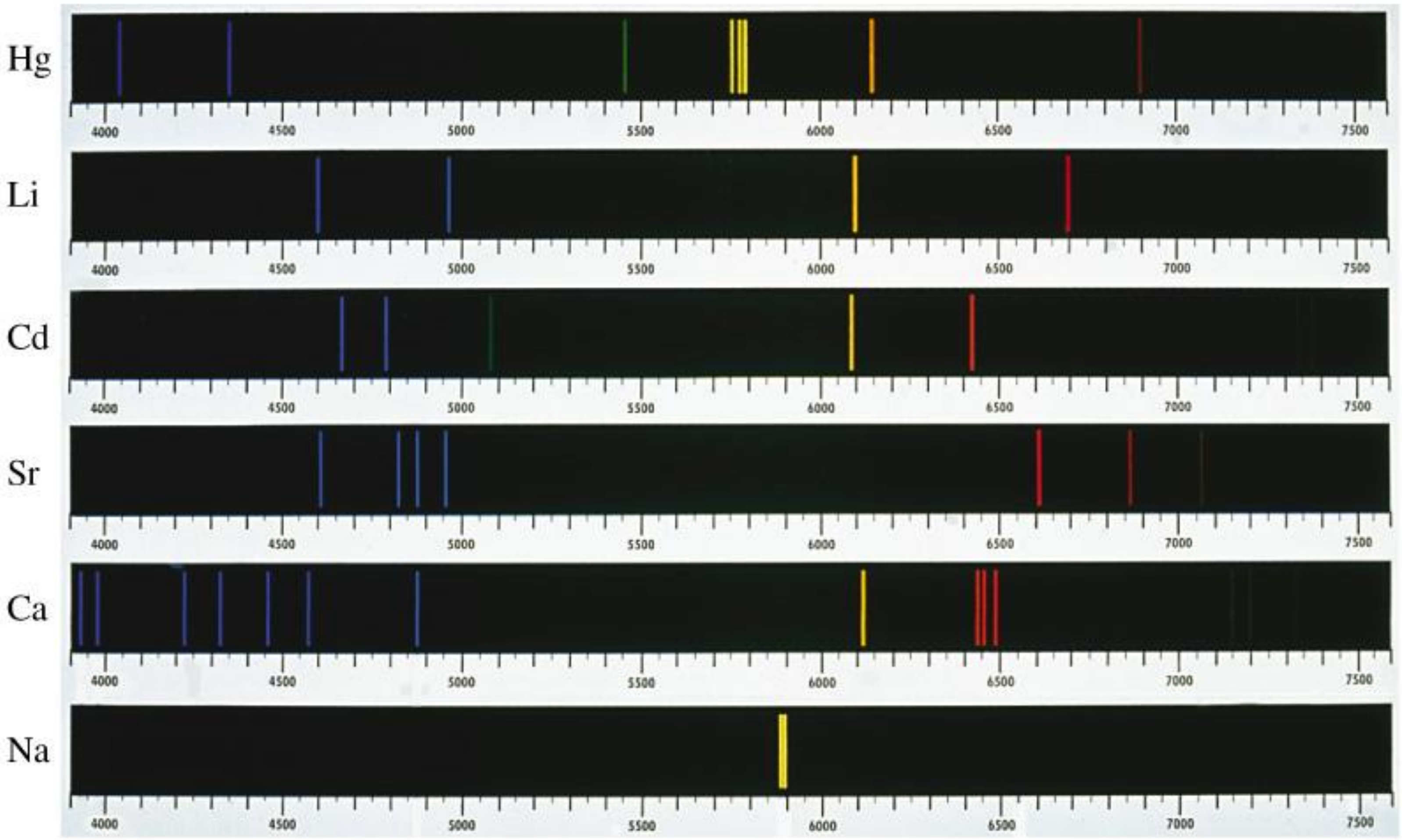


Quantum Theory of Atomic Structure



Quantum Theory of Atomic Structure

- The atomic emission spectra of gaseous *mercury*, *lithium*, *cadmium*, *strontium*, *calcium* and *sodium*:

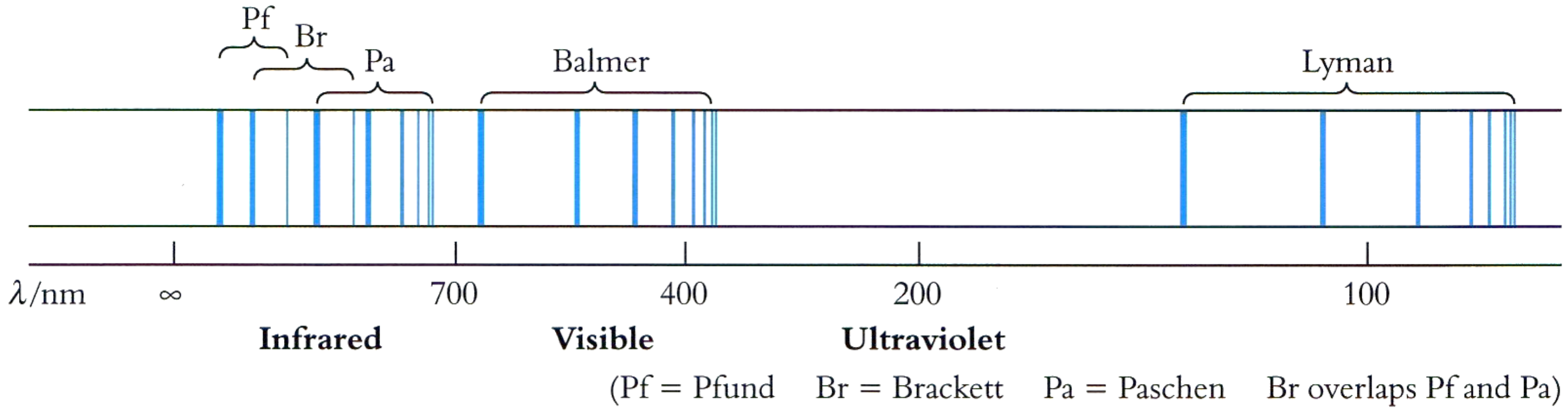


Quantum Theory of Atomic Structure

- The visible spectrum of *hydrogen* consists of 4 bands of light of specific wavelengths. This spectrum is generated when gaseous hydrogen is excited by an electrical current and the light given off by the gas is split by a prism.

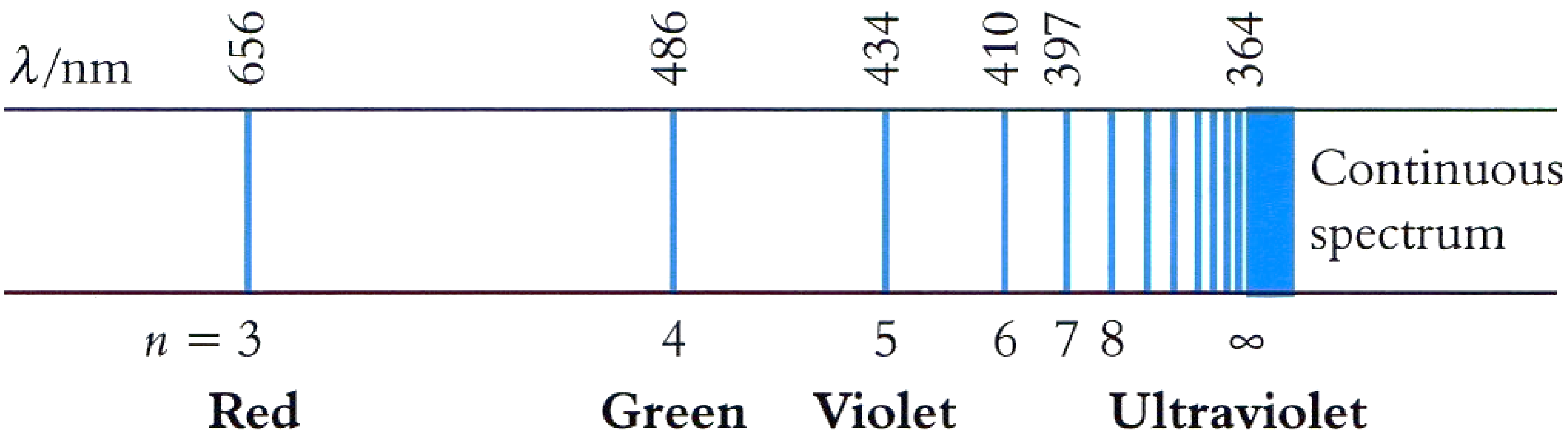
Quantum Theory of Atomic Structure

- Viewed through a *spectrometer*, the emission spectrum of hydrogen is seen to be a number of separate sets of lines, or a *series* of lines. Each series of lines is named after the scientist who discovered them as shown in the diagram below:



Quantum Theory of Atomic Structure

- A more detailed view of the *Balmer* series of hydrogen is shown in the diagram below:



- Note how the intervals between the frequencies of the lines becomes smaller and smaller towards the higher frequency end of the spectrum until the lines *converge together* to form a *continuous spectrum* of light.

Quantum Theory of Atomic Structure

- Why do atoms absorb or emit light of certain frequencies?
- Why do atomic spectra consist of discrete (separate) lines?
- Why do the spectral lines converge at higher frequencies to form a continuous spectrum?

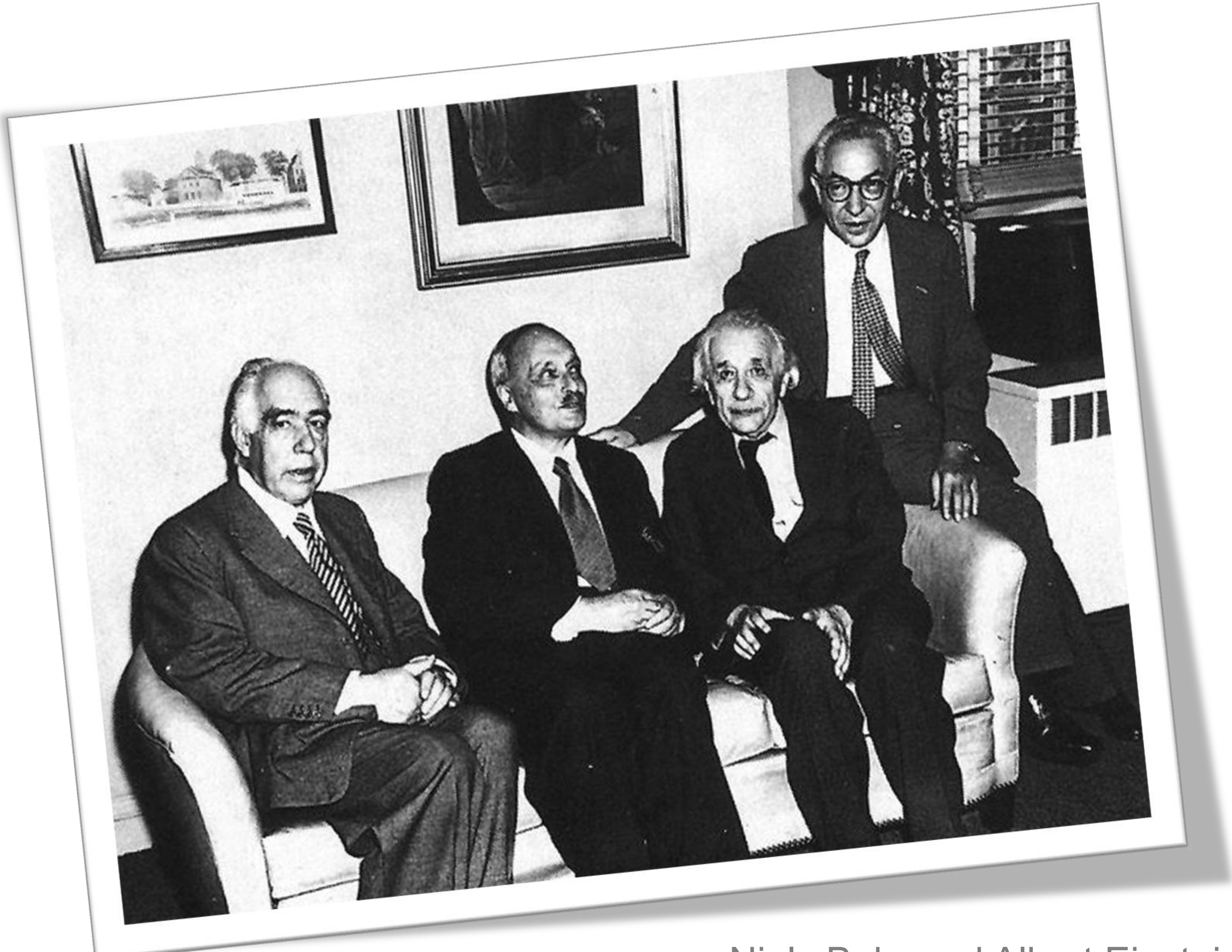
Quantum Theory of Atomic Structure

- Niels Bohr (1885 – 1962) Nobel Prize for Physics 1922.

- In 1913, *Niels Bohr* put forward his structure of the atom to answer these questions. Bohr referred to *Max Planck's* recently discovered *quantum theory*, according to which energy can be absorbed or emitted in certain amounts, like separate packets of energy, called *quanta*.

- Max Planck (1858 – 1947) Nobel Prize for Physics 1918.

Quantum Theory of Atomic Structure



- Niels Bohr and Albert Einstein.

Quantum Theory of Atomic Structure

- Niels Bohr suggested the following:

1) An electron moving in an orbit can only have certain amounts of energy, not an infinite number of values, *i.e.* the electron's energy is *quantised*.

2) The energy that an electron needs to move in a particular orbit depends upon the radius of the orbit. An electron that is moving in an orbit *distant* from the nucleus has a *higher* energy compared to an electron that is moving in an orbit near to the nucleus of the atom.

Quantum Theory of Atomic Structure

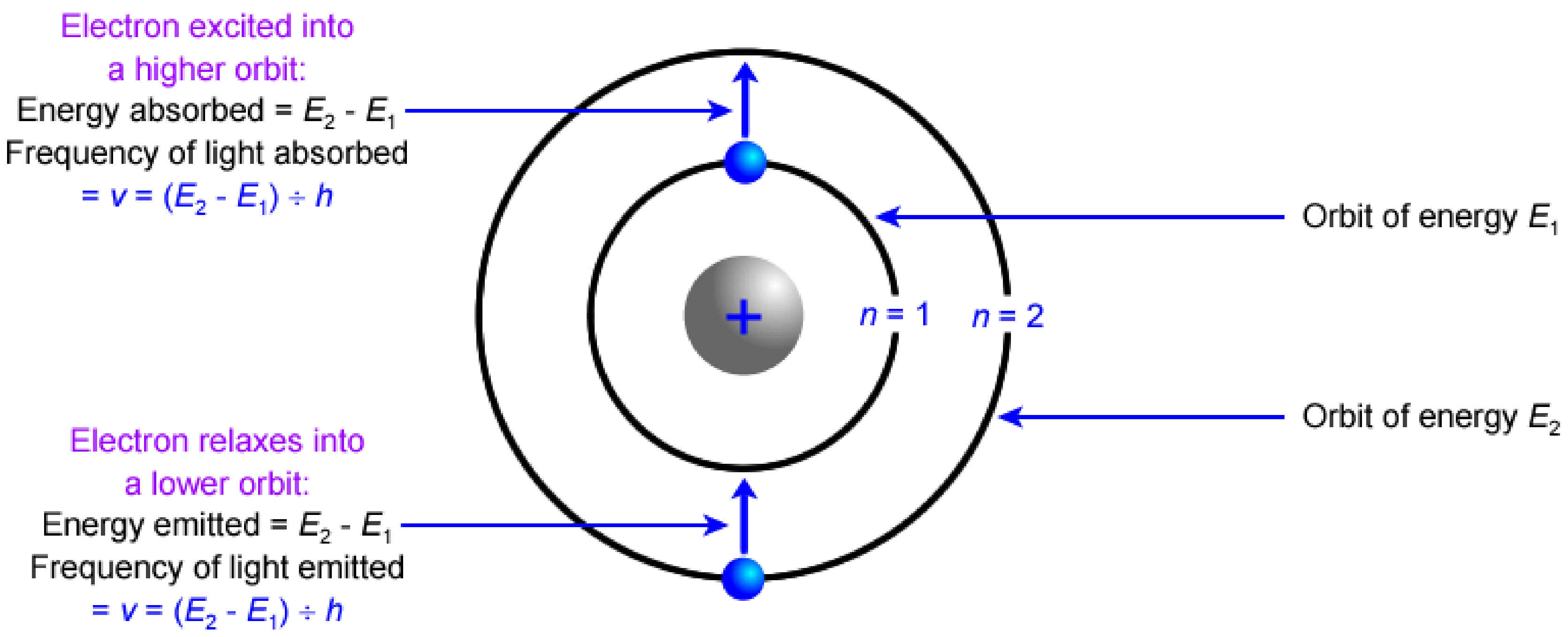
3) If the energy of the electron is quantised, then the radius of the orbit must also be quantised. An atom therefore contains a restricted number of orbits, not an infinite number of orbits.

4) An electron moving in one of these orbits does not emit energy. In order to move to an orbit further away from the nucleus, the electron must *absorb* energy to do work against the attraction of the nucleus. If an atom absorbs a *photon* of light, then the absorbed energy can promote (*excite*) an electron from an inner orbit to an outer orbit. When an electron falls (*relax*) from a higher orbit to a lower orbit, then energy is *released* as a photon of light.

Quantum Theory of Atomic Structure

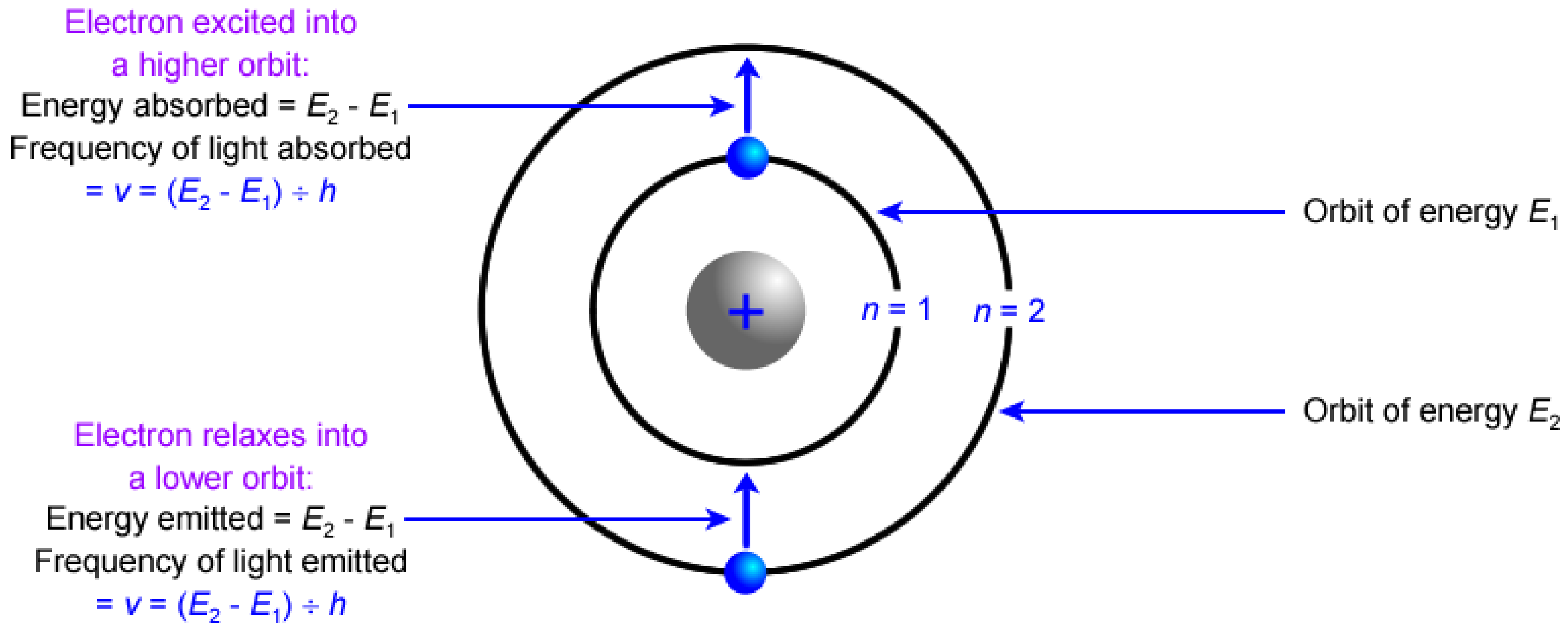
- For an electron to move from an orbit of energy E_1 to E_2, the light absorbed must have a frequency given by *Planck's equation*:

$hv = E_2 - E_1$ where v = frequency and h = Planck's constant.



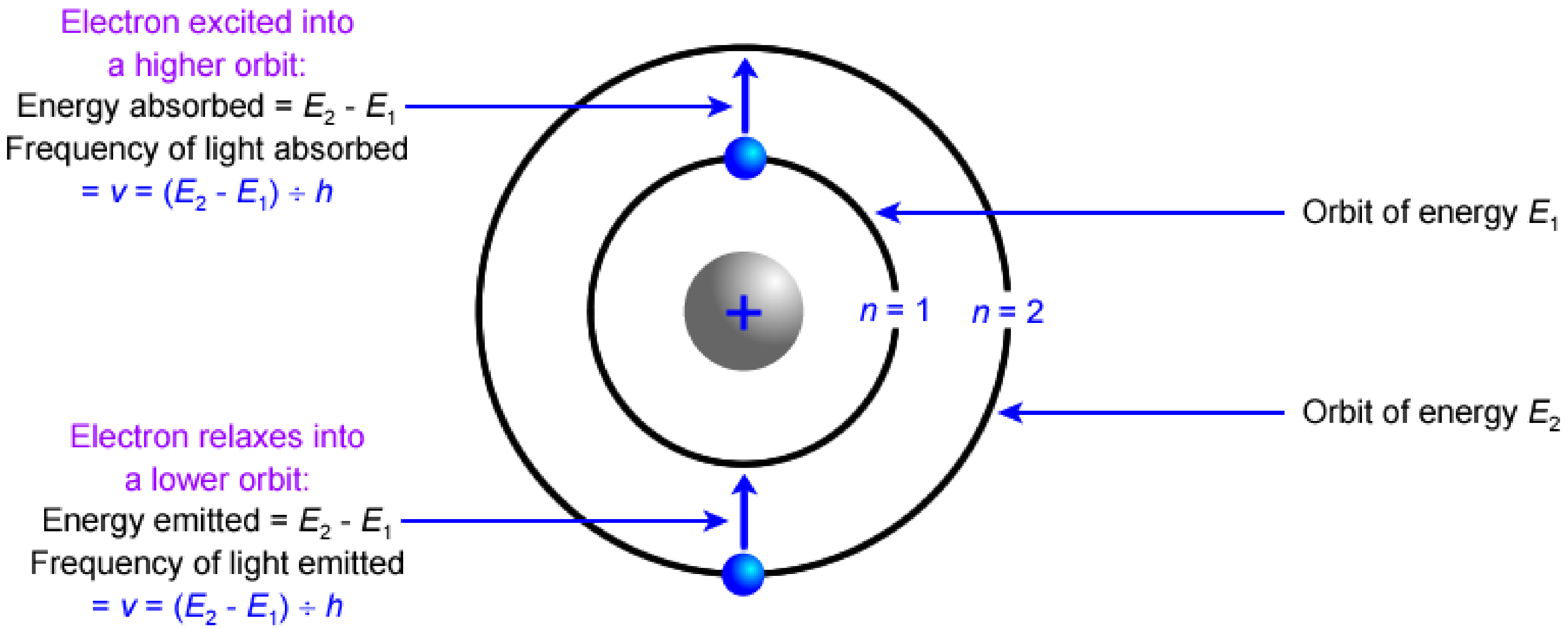
Quantum Theory of Atomic Structure

- The emission spectrum arises when electrons which have been excited (raised into orbits of higher energy) fall back to orbits of lower energy. As these electrons relax, they emit energy as light with a frequency given by Planck's equation.

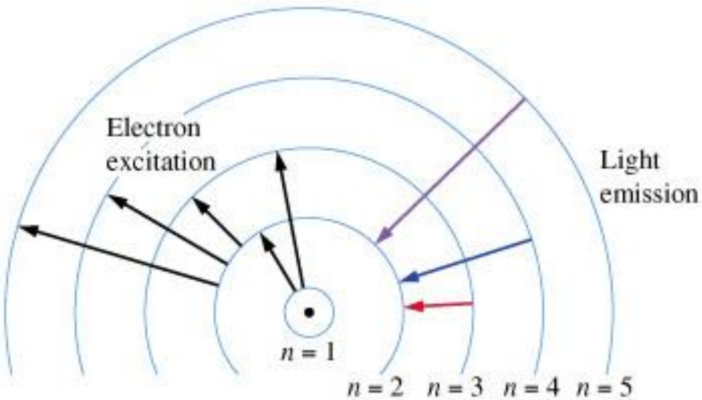


Quantum Theory of Atomic Structure

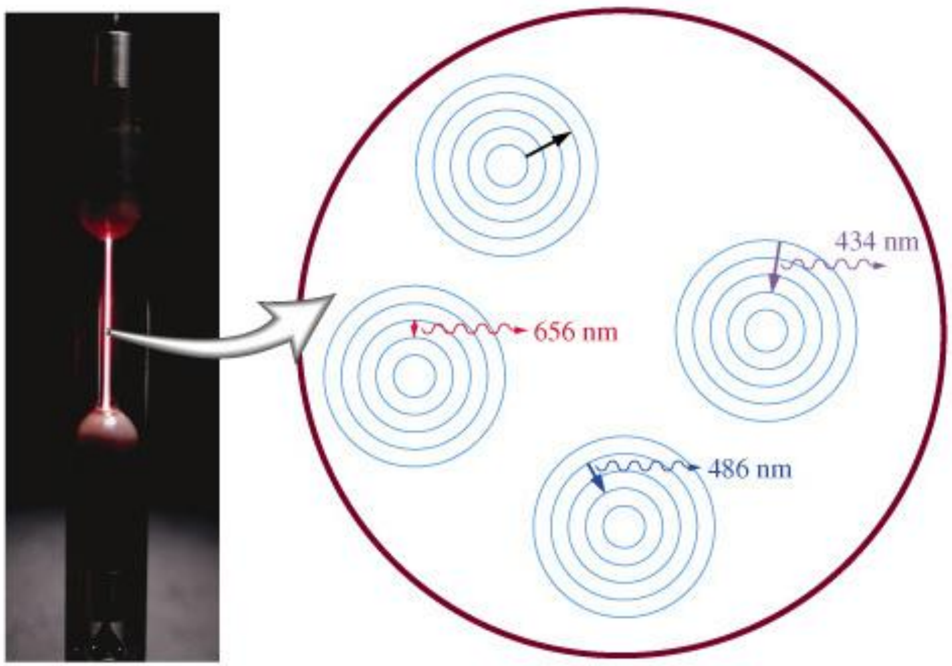
- Bohr assigned *quantum numbers* to the orbits. He gave the orbit of lowest energy (closest to the nucleus) the quantum number *1*. An electron in this orbit is said to be in its *ground state*. The next energy level has a quantum number of 2.



Quantum Theory of Atomic Structure



(a)

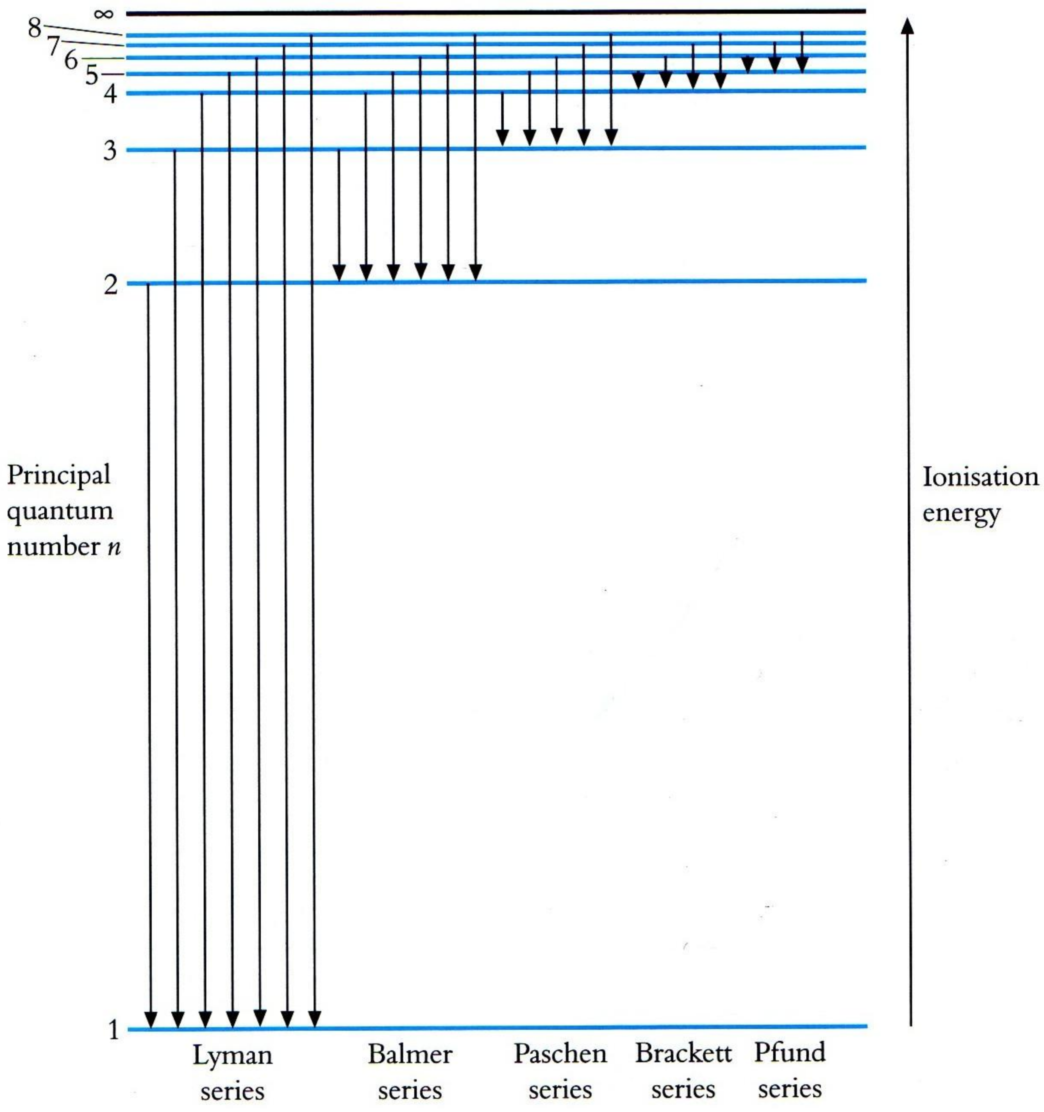


(b)

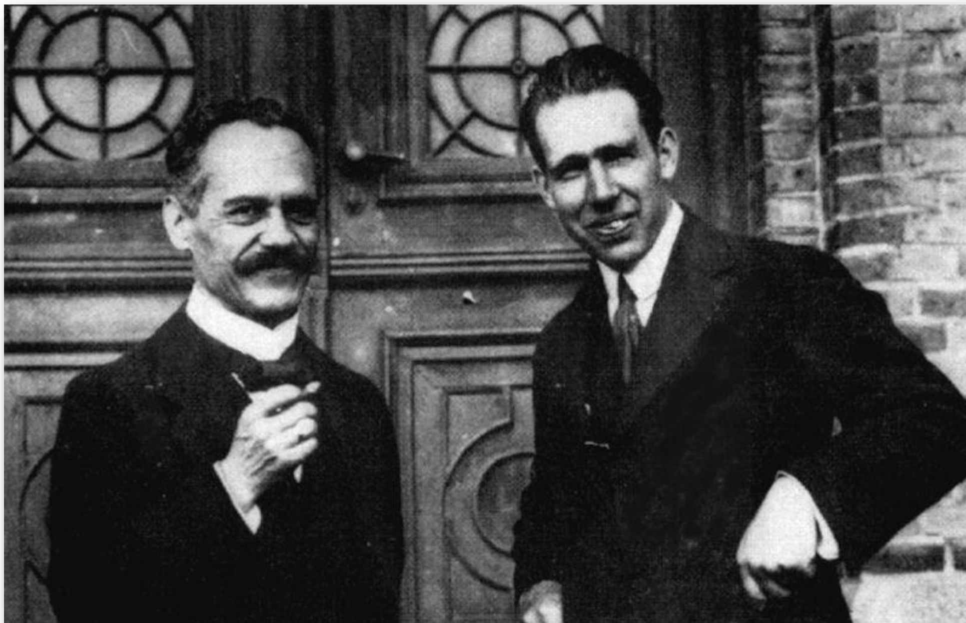
- The emission spectrum of hydrogen arises when the electron in its ground state absorbs energy and is excited into a higher energy orbit. When the electron relaxes into a lower energy orbit, it releases energy as light with a frequency given by Planck's equation:

$$hv = E2 - E1$$

Quantum Theory of Atomic Structure



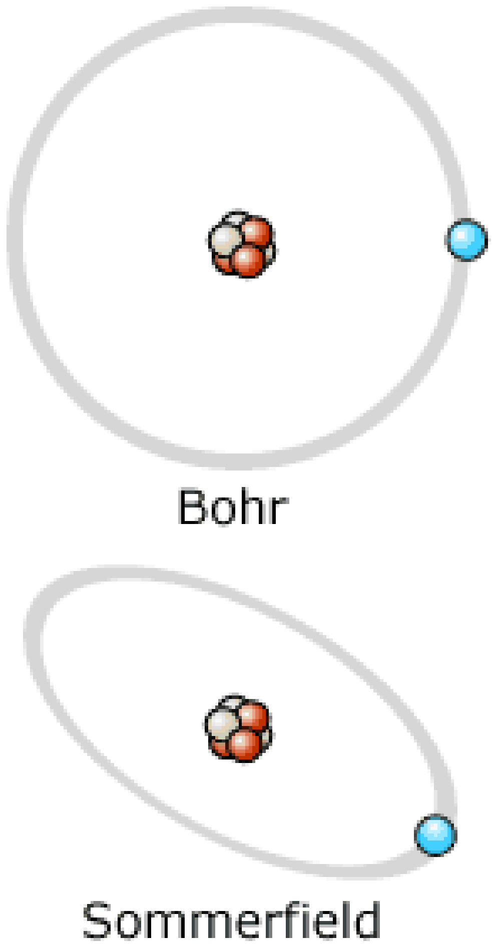
Quantum Theory of Atomic Structure



• Arnold Sommerfeld (1868 – 1951) and Niels Bohr.

• *Arnold Sommerfeld* elaborated on Bohr's theory in1916. He proposed that each quantum number governed the energy of a circular orbit and also a set of *elliptical orbits* of similar energy.

Quantum Theory of Atomic Structure



- Sommerfeld also called *n* the *principle quantum number* and introduced a second quantum number to describe the shapes of the elliptical orbits.
- The second quantum number, *l*, can have values from (*n* – *1*) down to *0*. For example, if *n* = *4*, then the values of *l* would be *3*,*2*,*1* and *0*.

Quantum Theory of Atomic Structure

• Louis de Broglie
(1892 – 1987)
Awarded the Nobel Prize for Physics in 1929.

• According to the wave theory of light, refraction and diffraction can be explained by the properties of waves. Other properties of light, such as the origin of line spectra and the photoelectric effect need a particle or photon theory for their explanation. The success of the duel theory of light led *Louis de Broglie* to speculate in 1924 on whether particles might have wave properties. He made the bold suggestion that *electrons have wave properties* as well as the *properties of particles*.

Schrödinger's Wave Equation

- Erwin Schrödinger
(1887 – 1961)
Awarded the Nobel Prize
for Physics in 1933.

- Paul Dirac
(1902 – 1984)
Awarded the Nobel Prize
for Physics in 1933.

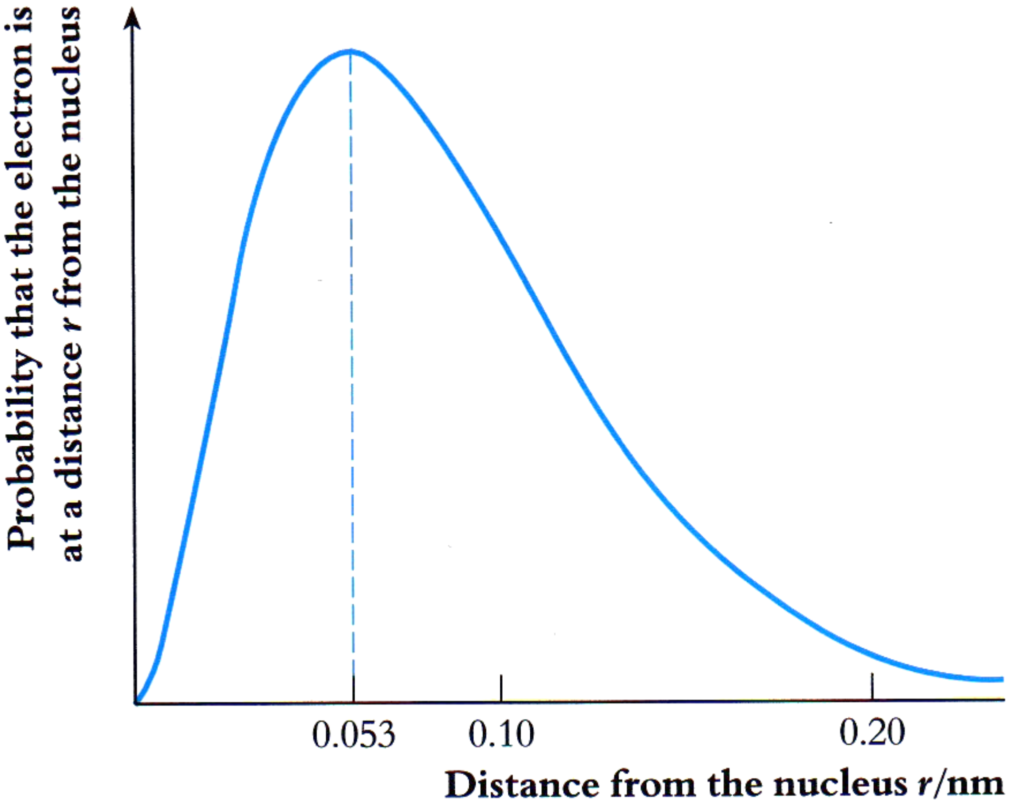
Schrödinger's Wave Equation

- *Erwin Schrödinger* and *Paul Dirac* used de Broglie's theory to work out a wave theory for the atom. One version of Schrödinger's famous wave equation is given below:

$$\frac{\delta^2\Psi}{\delta x^2} + \frac{\delta^2\Psi}{\delta y^2} + \frac{\delta^2\Psi}{\delta z^2} + \frac{8m\pi^2}{h^2}(E - V)\Psi = 0$$

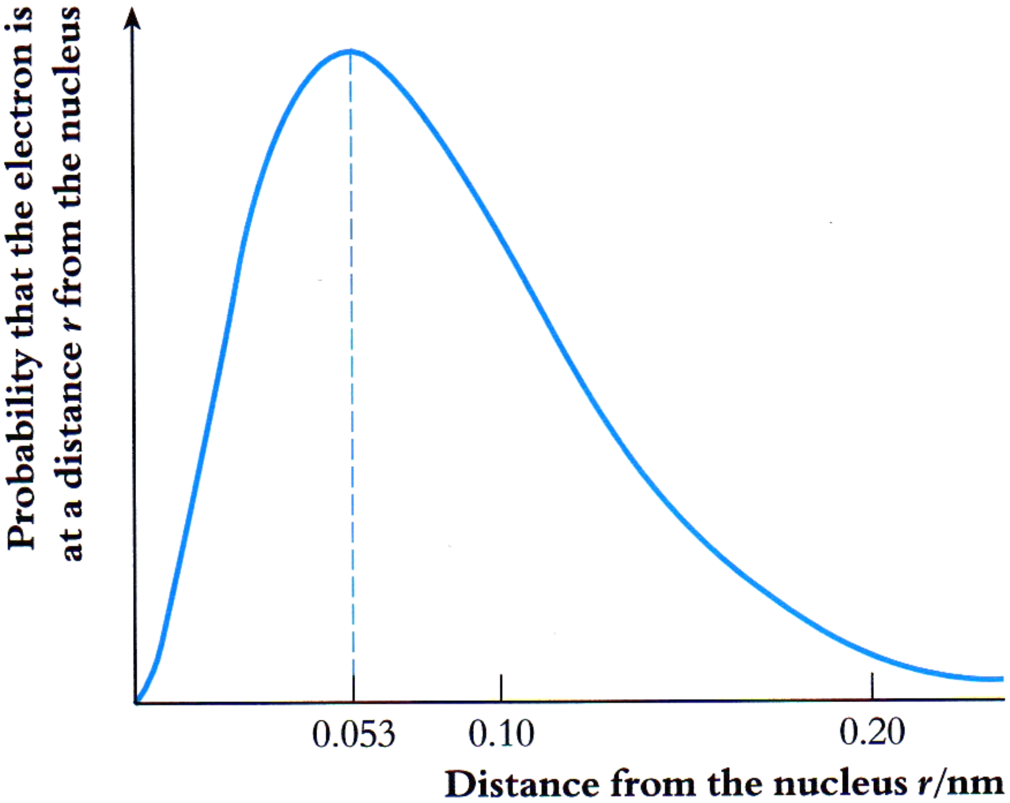
- The solution to the wave equation gives the *probability density* of the electron. This is the probability that the electron is present in a small given region of space.

Schrödinger's Wave Equation



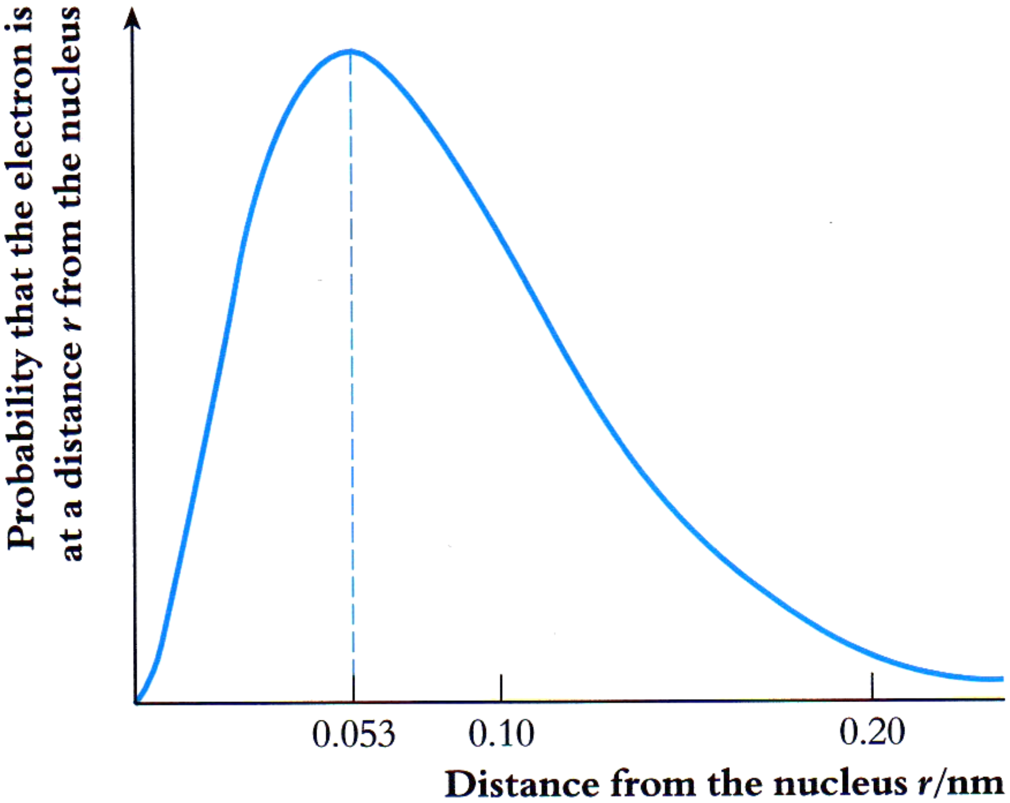
- The graph on the left shows a probability density diagram for a hydrogen atom in its ground state. The maximum probability of finding an electron is *0.053 nm* from the nucleus.

Schrödinger's Wave Equation



- There is a possibility that the electron will be either closer to the nucleus or outside the radius of 0.053 nm. The probability of finding the electron decreases sharply as the distance from the nucleus increases beyond *3r*.

Schrödinger's Wave Equation



- The volume of space in which there is a *95%* probability of finding the electron is called the *atomic orbital*.

Schrödinger's Wave Equation

- Solutions of the wave equation can be obtained if the orbitals are described by *four quantum numbers*.

- The first is Bohr's principle quantum number, *n*.

- The second quantum number, *l*, corresponds to Sommerfeld's quantum number describing the shape of the elliptical orbits. The values of *l* are assigned letters:

l = 0 = s
l = 1 = p
l = 2 = d
l = 3 = f

Schrödinger's Wave Equation

- If an electron has a principle quantum number $n = 2$ and a second quantum number $l = 0$, it is said to be a *2s* electron. For various values of n, the different combinations of the two quantum numbers are:

1s
2s   *2p*
3s   *3p*   *3d*
4s   *4d*   *4d*   *4f*

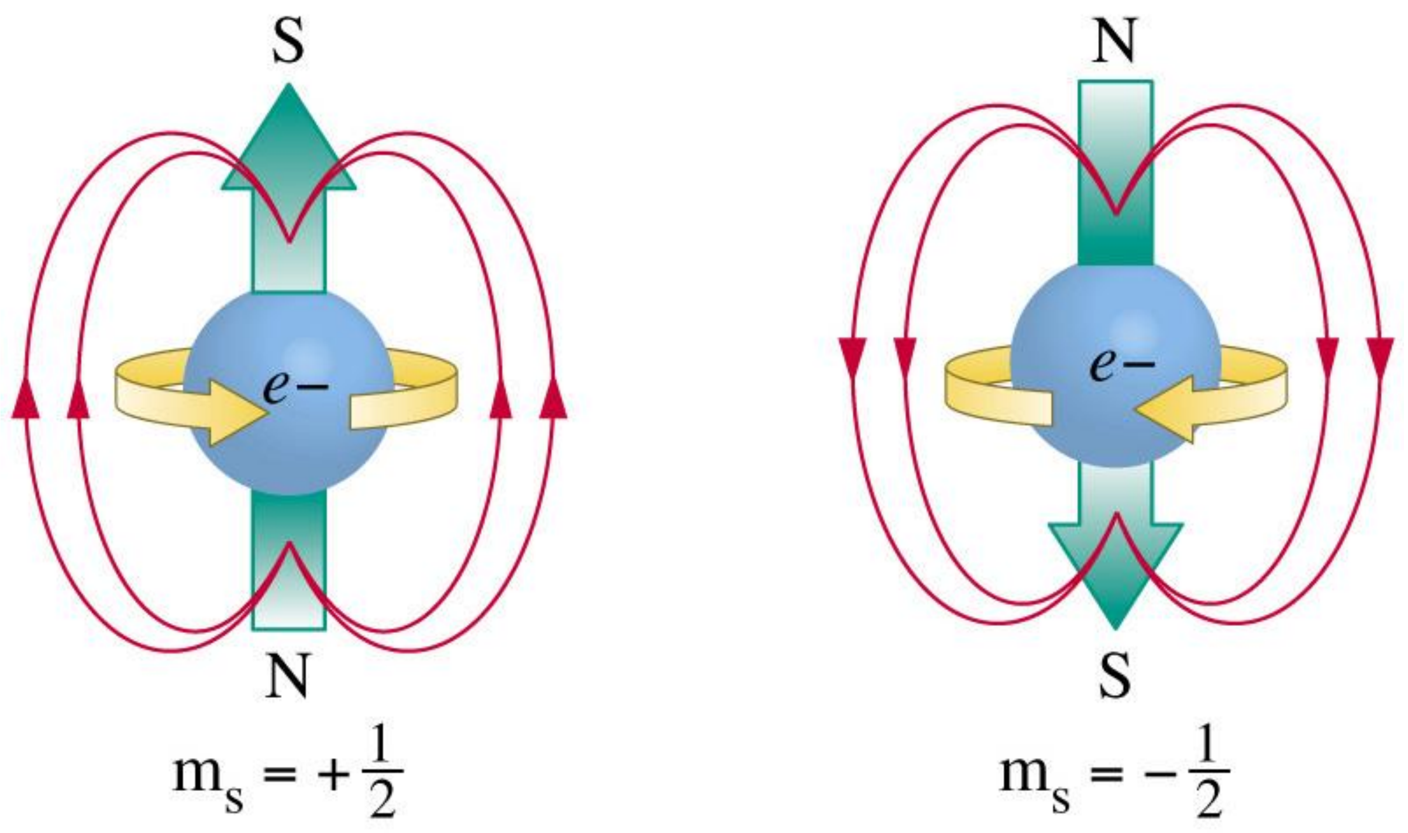
Schrödinger's Wave Equation

- Schrödinger's wave equation leads to a third quantum number, m_l. This gives the maximum number of orbitals for the different values of l:

One s-orbital
Three p-orbitals
Five d-orbitals
Seven f-orbitals

Schrödinger's Wave Equation

- The fourth quantum number is called the *spin quantum number*, m_s. It has values of $+\frac{1}{2}$ and $-\frac{1}{2}$ and represents the spin of the electron on its own axis.



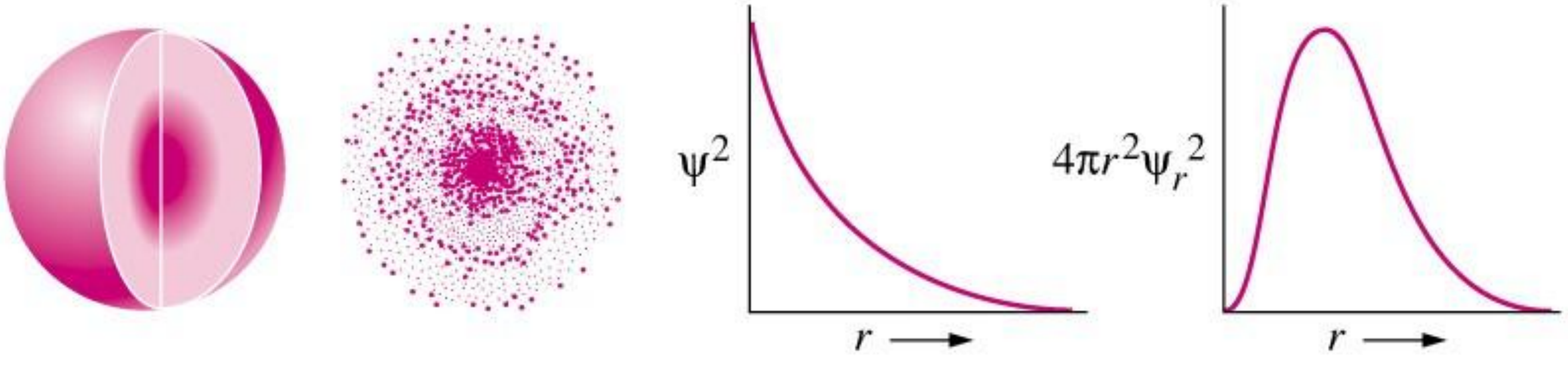
Schrödinger's Wave Equation

- Wolfgang Pauli (1900 – 1958) Awarded the Nobel Prize for Physics in 1945.

- Pauli's exclusion principle states that *no two electrons in an atom can have the same four quantum numbers*. It therefore follows that if two electrons in an atom have the same values of n, l, and m_l, they must have different values of m_s, *i.e. their spins must be opposed*. The consequence of this is that an orbital can hold a maximum number of *two electrons* with *opposite spins*.

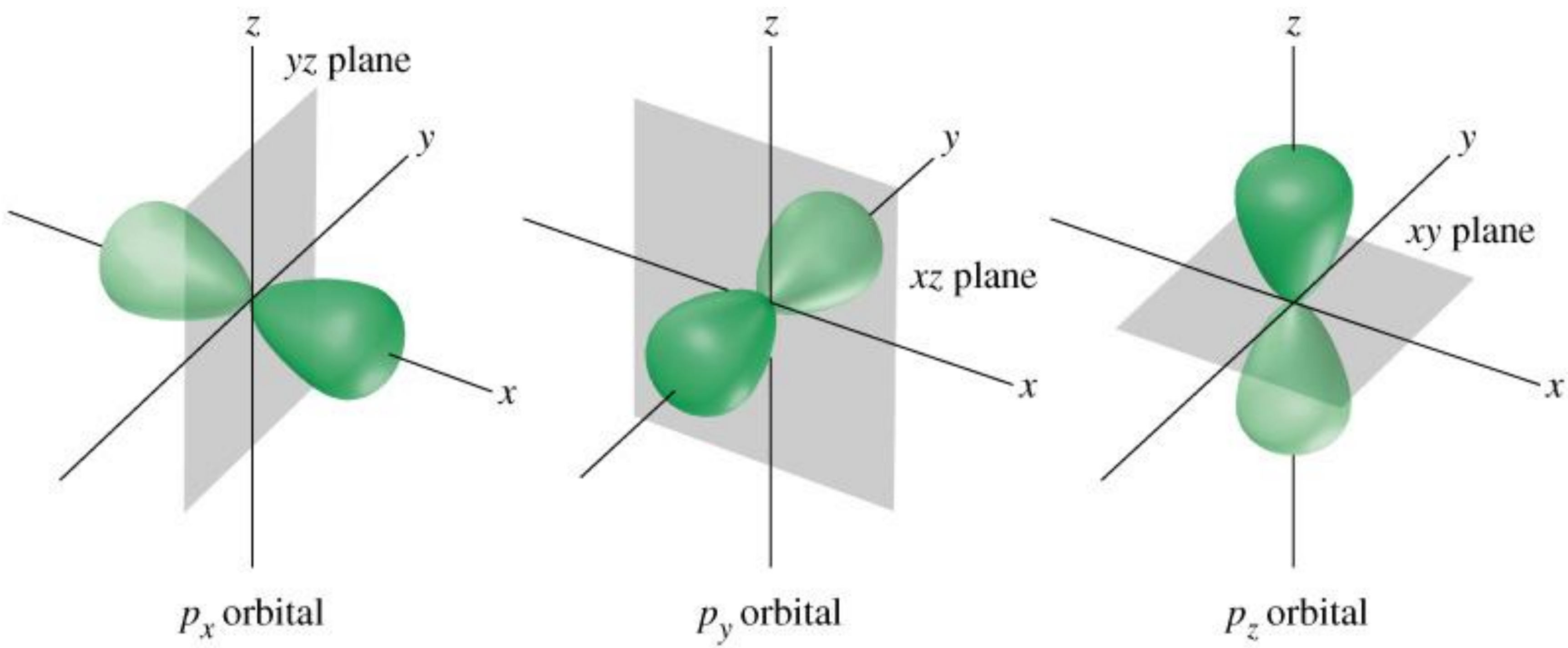
Schrödinger's Wave Equation

- The shape of an *s-orbital* is *spherically symmetrical* about the nucleus. The orbital has no preferred direction. The probability of finding an electron at a distance *r* from the nucleus is the same in all directions.



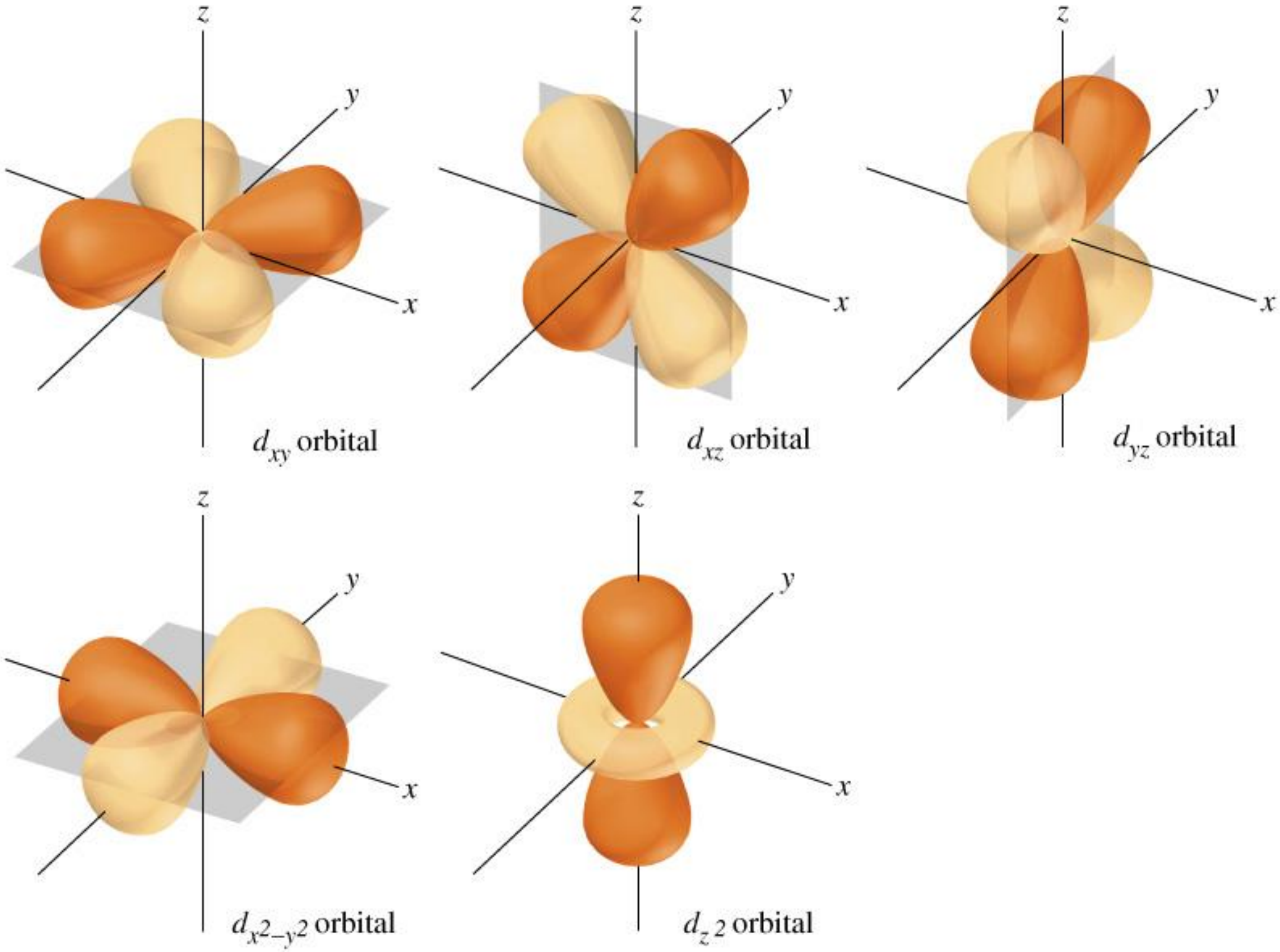
Schrödinger's Wave Equation

- A *p-orbital* is concentrated in certain directions. *p-orbitals* exits in groups of *three* arranged at 90° to each other.

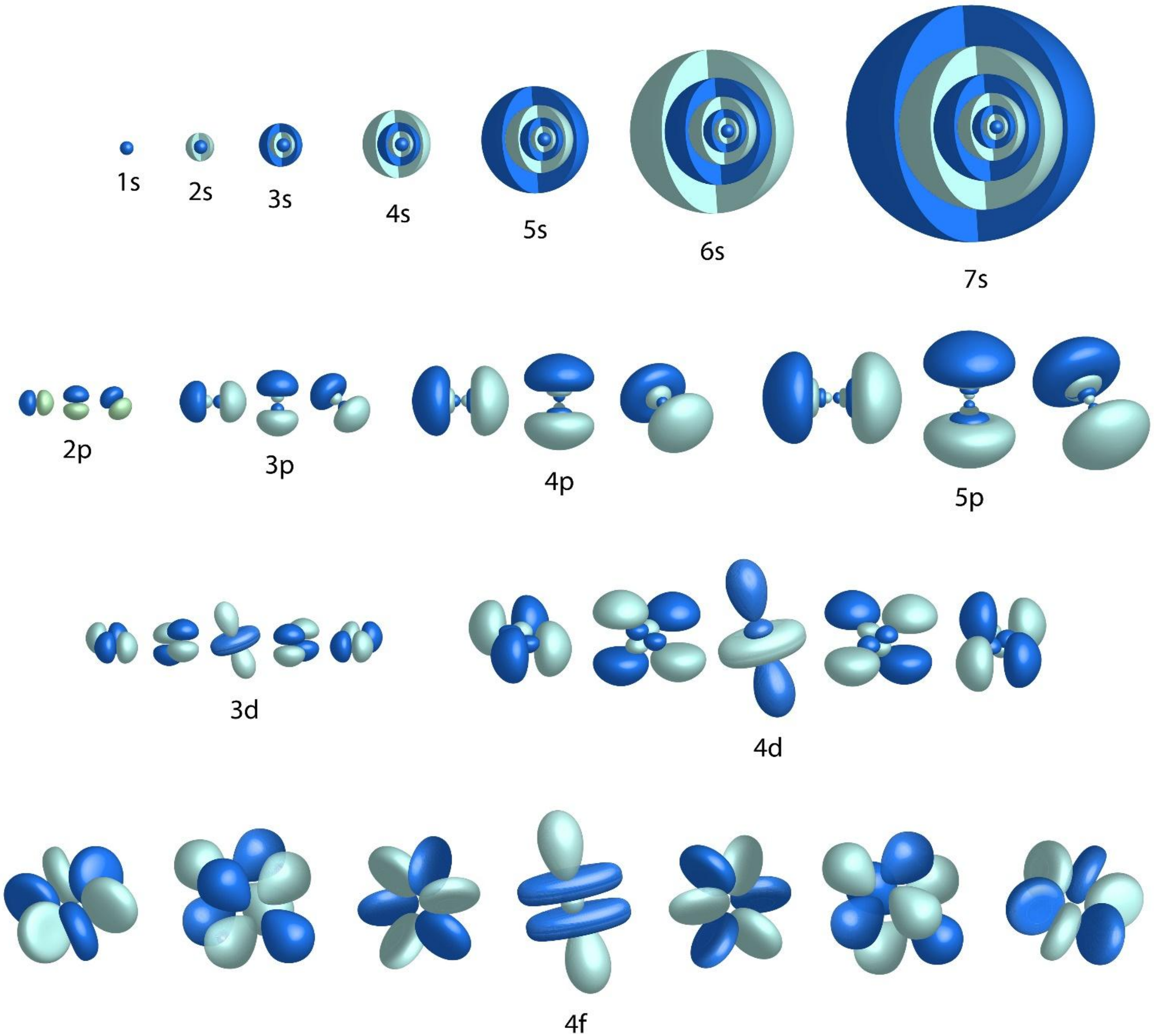


Schrödinger's Wave Equation

- *d-orbitals* are arranged in groups of *five*.



Schrödinger's Wave Equation



Electronic Configurations

- The term *shell* is used for a group of orbitals with the same principle quantum number (*n*). A *sub-shell* is a group of orbitals with the same principle and second quantum numbers (*n* and *l*), *e.g.* the *3p subshell*.

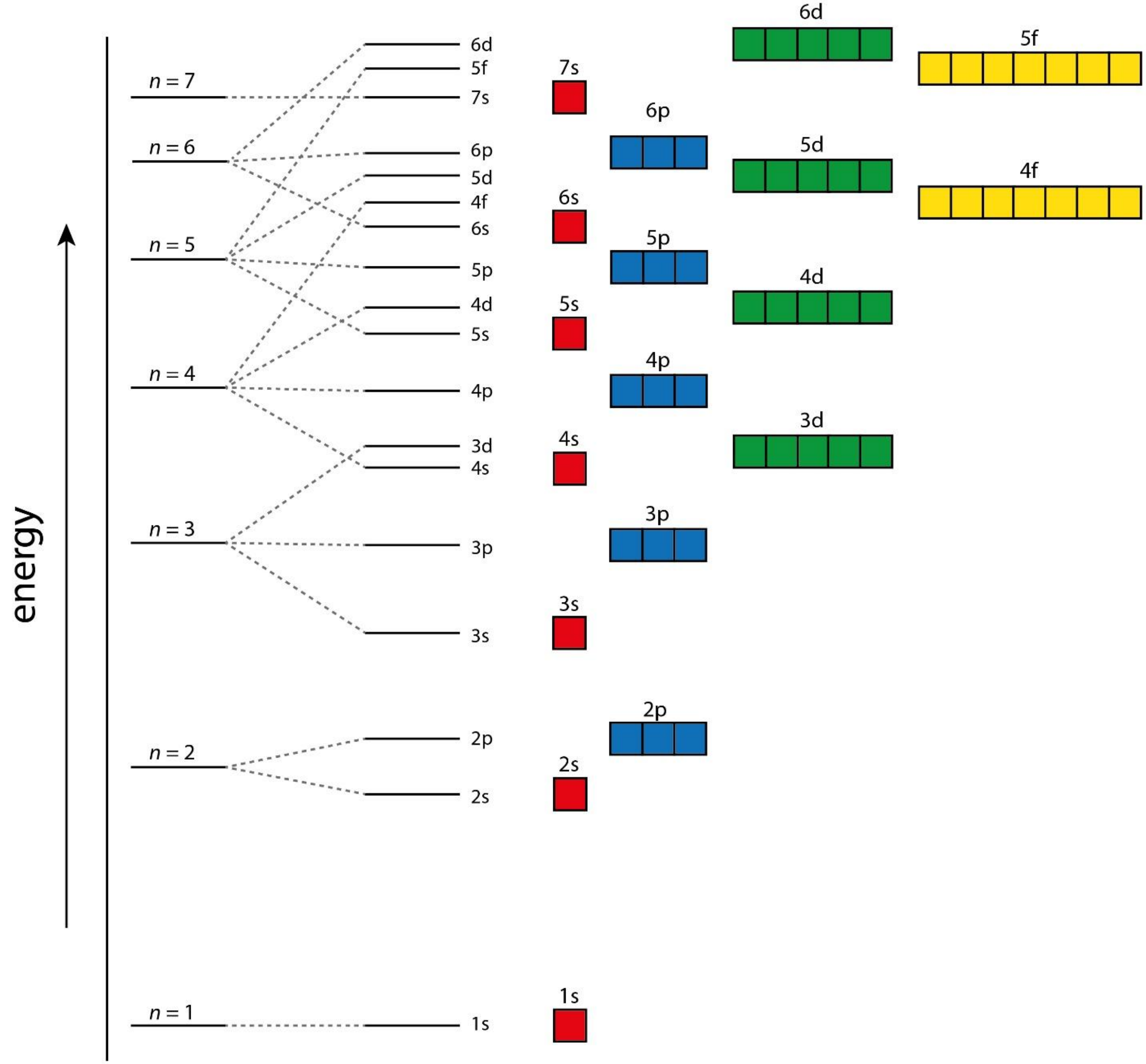
- When writing out the electron configurations of atom, it is convenient to remember the following:

→ Electrons should fill orbitals from the *lowest energy* to the *highest energy* (known as the *Aufbau principle*).

→ The Pauli Exclusion Principle – no two electrons in the same atom can have the same four quantum numbers.

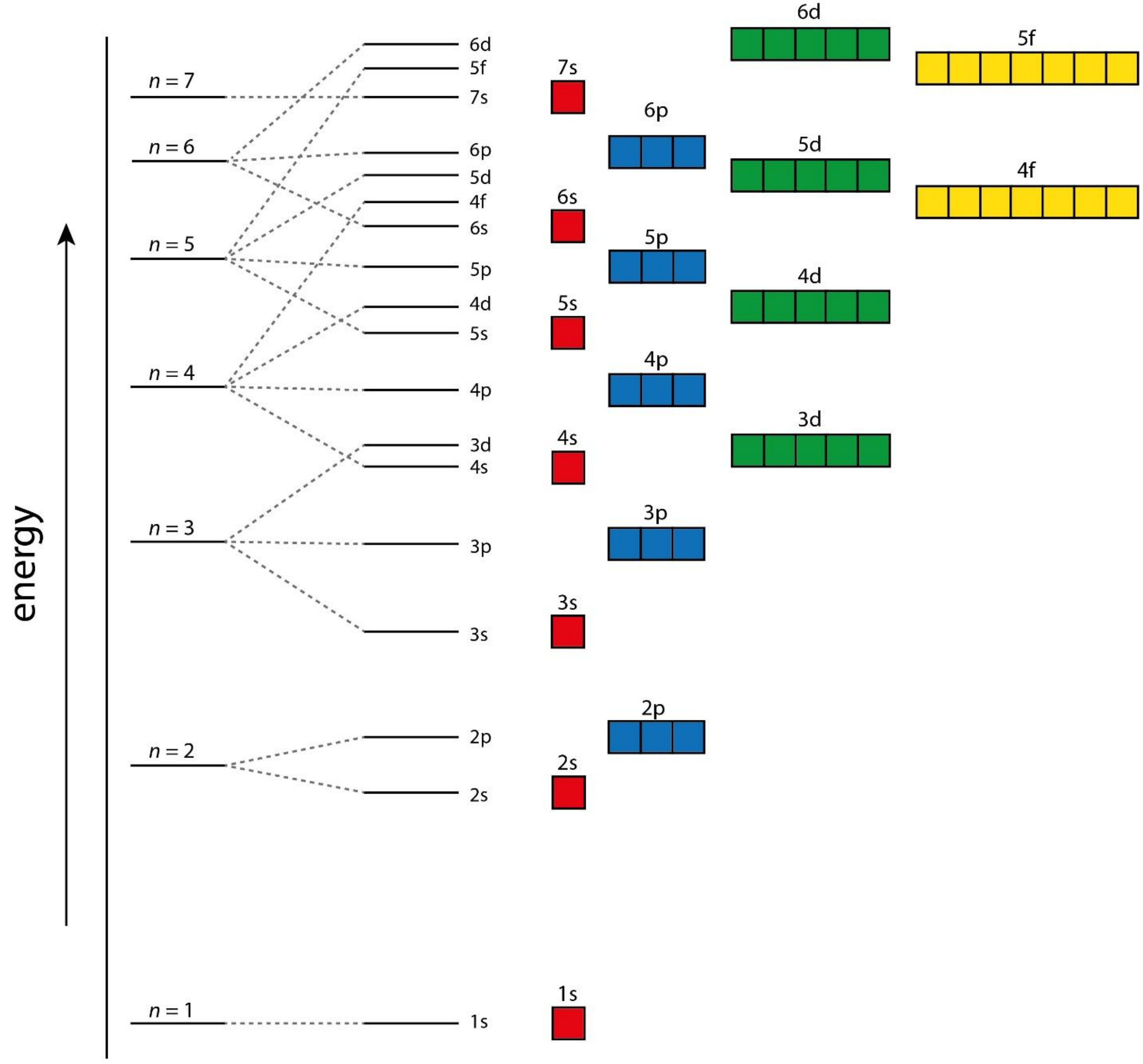
→ Orbitals fill-up in the order *1s*, *2s*, *2p*, *3s*, *3p*, *4s*, *3d*, *4p*.

Electronic Configurations



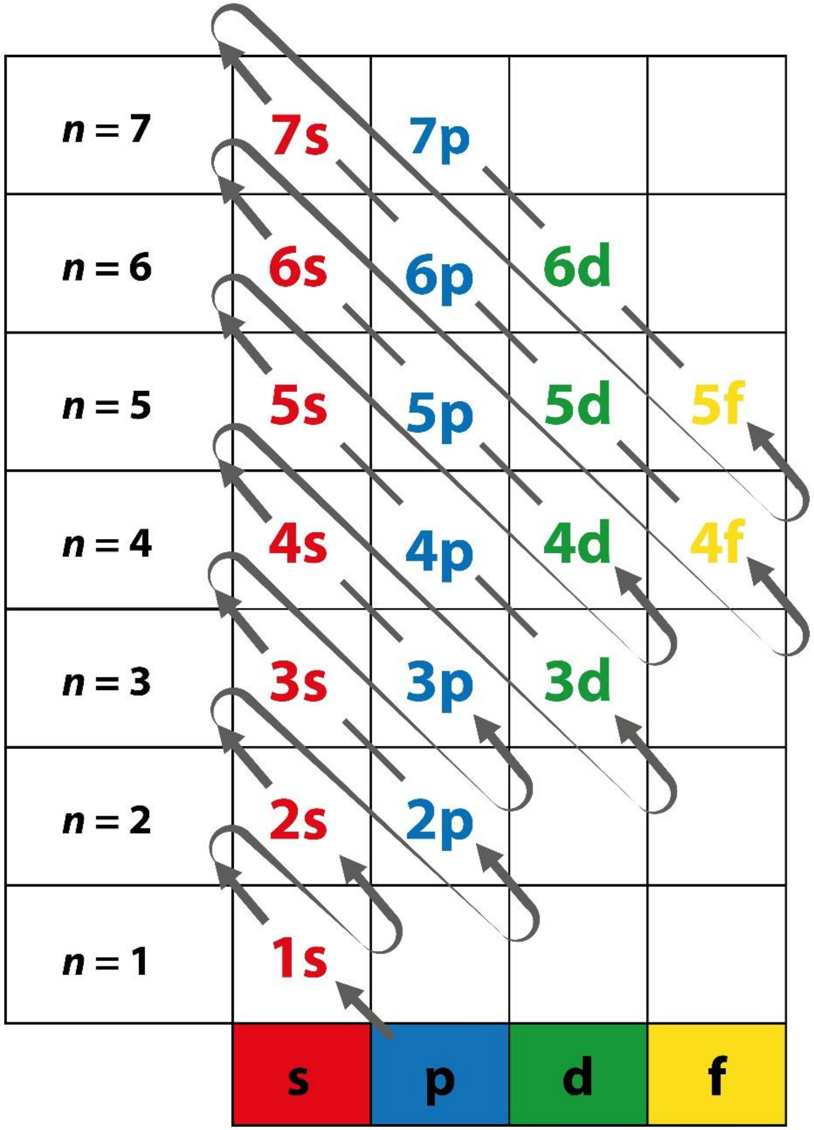
- For convenience, orbitals are often drawn as *boxes*.
- Each orbital can hold a maximum number of *two electrons*. These are represented by drawing arrows in the boxes, one arrow pointing up and one arrow pointing down to represent the opposite spin.

Electronic Configurations



- *s-orbitals* (red) are represented by a single box.
- *p-orbitals* (blue) are represented by a group of three boxes.
- *d-orbitals* (green) are represented by a group of five boxes.

Electronic Configurations



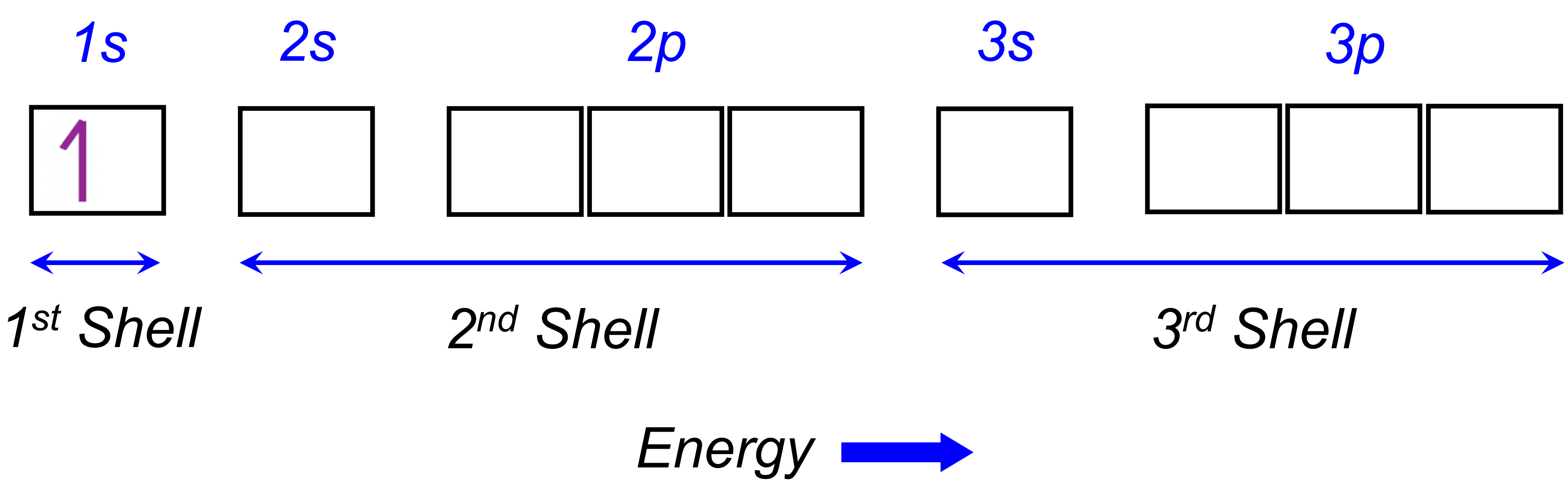
- This diagram shows the order in which the orbitals fill-up, from the lowest energy to the highest energy.

et cetera
3d
↑
4s
↑
3p
↑
3s
↑
2p
↑
2s
↑
1s

Electronic Configurations

- It is convenient to draw "*electrons in boxes*" diagrams to show the arrangement of electrons in orbitals. Arrows are used to represent the electrons. Arrows pointing in opposite directions represent electrons with *opposite spin*.

1 – Hydrogen



Electronic Configurations

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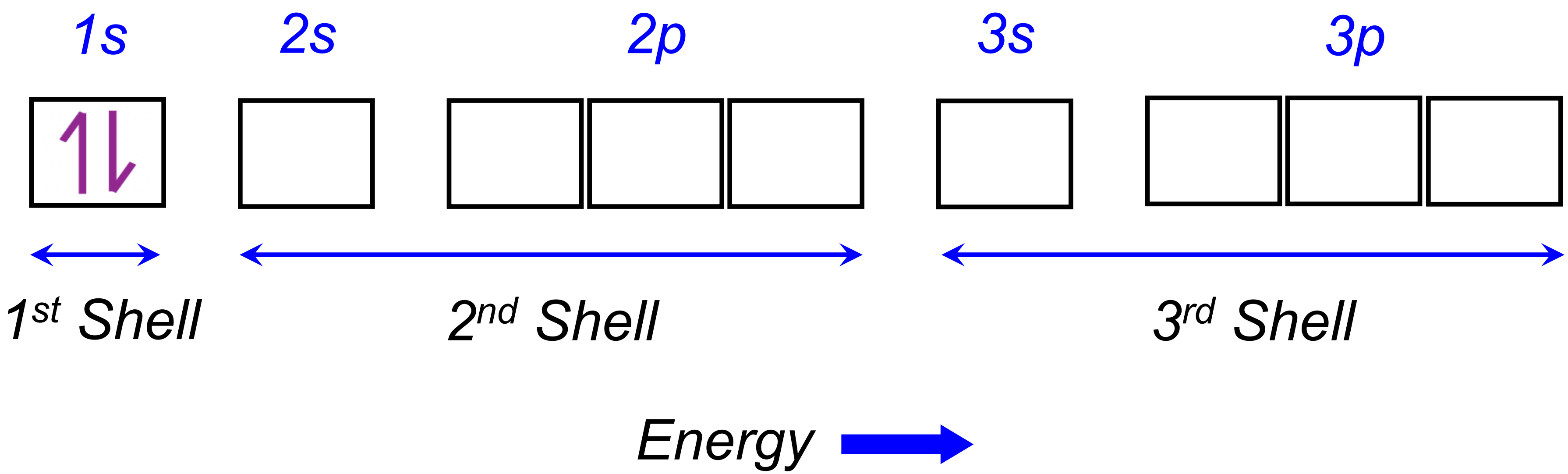
2 – Helium



Electronic Configurations

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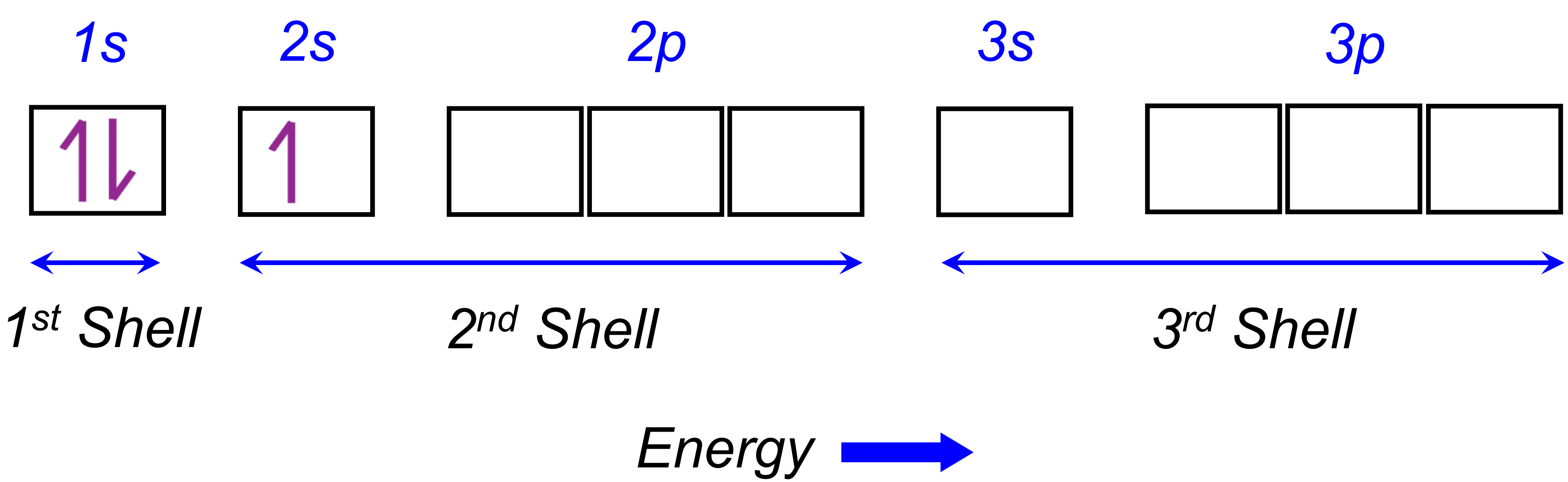
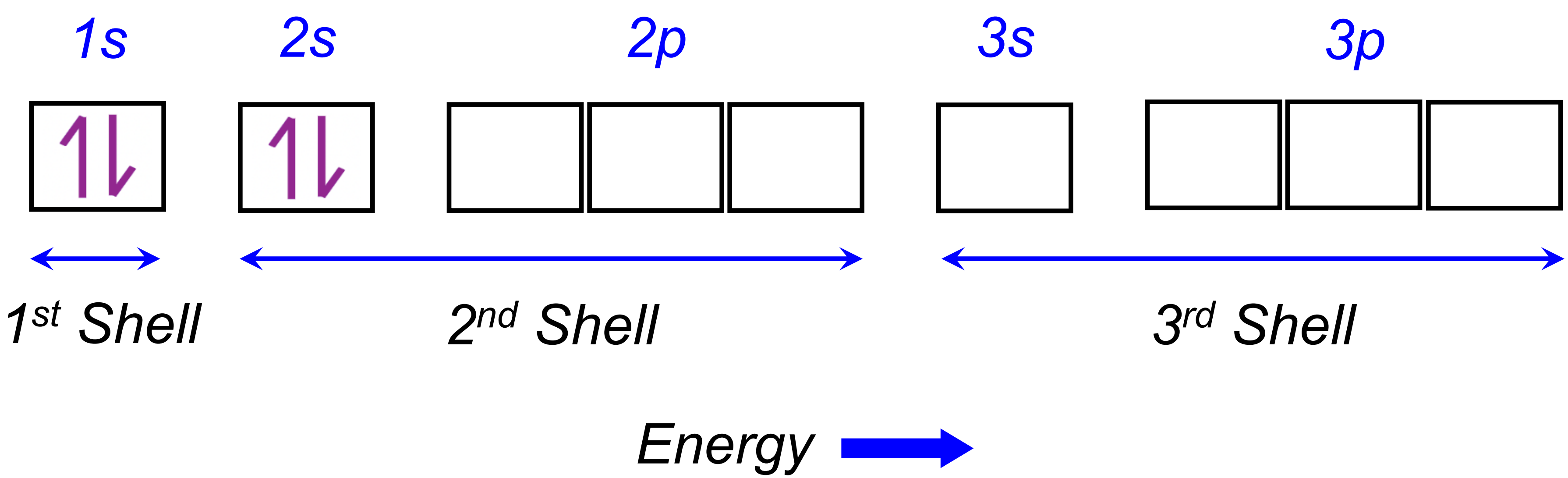
3 – Lithium



Electronic Configurations

- It is convenient to draw "*electrons in boxes*" diagrams to show the arrangement of electrons in orbitals. Arrows are used to represent the electrons. Arrows pointing in opposite directions represent electrons with *opposite spin*.

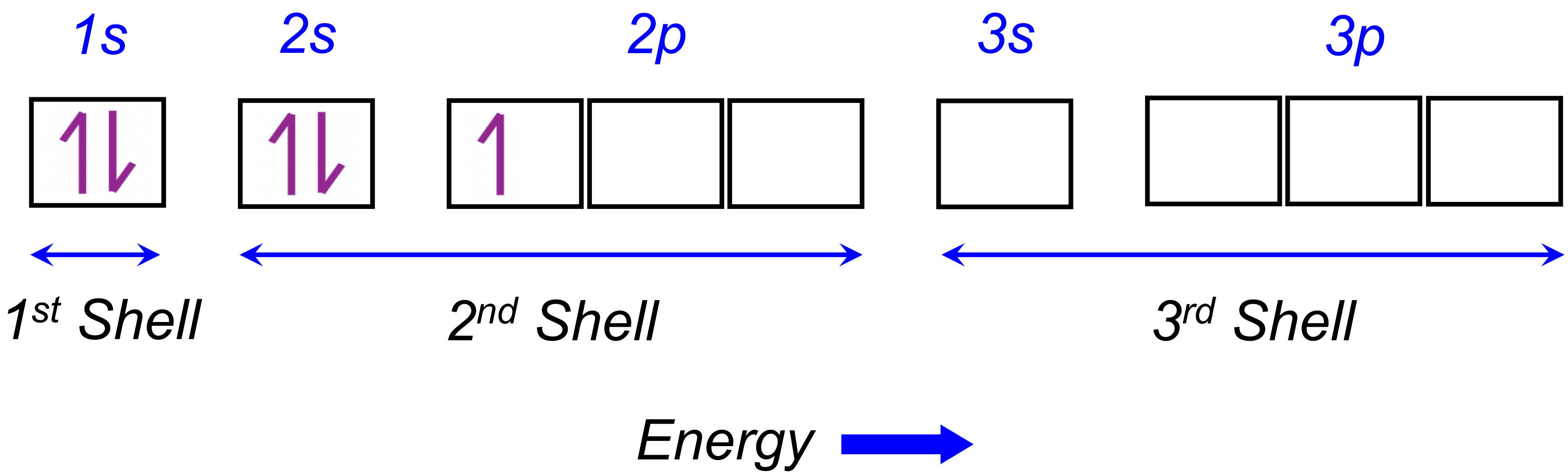
4 – Beryllium



Electronic Configurations

- It is convenient to draw "*electrons in boxes*" diagrams to show the arrangement of electrons in orbitals. Arrows are used to represent the electrons. Arrows pointing in opposite directions represent electrons with *opposite spin*.

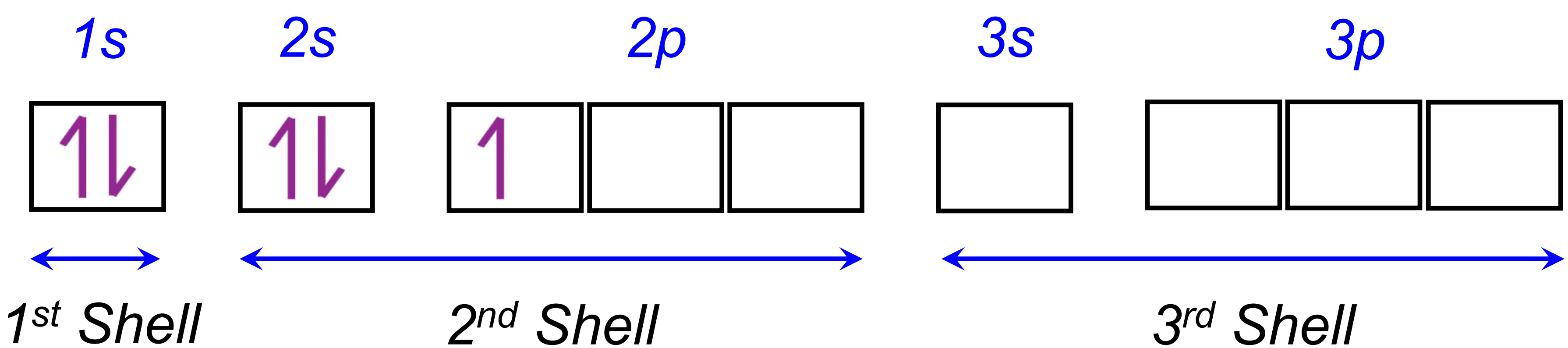
5 – Boron



Electronic Configurations

• Note: Because electrons all carry a charge of –1, they naturally repel each other. Because of this, when electrons enter p-orbitals, they will initially occupy separate p-orbitals before they are forced to pair-up (*spin-pair*) with each other.

5 – Boron



Energy →

Electronic Configurations

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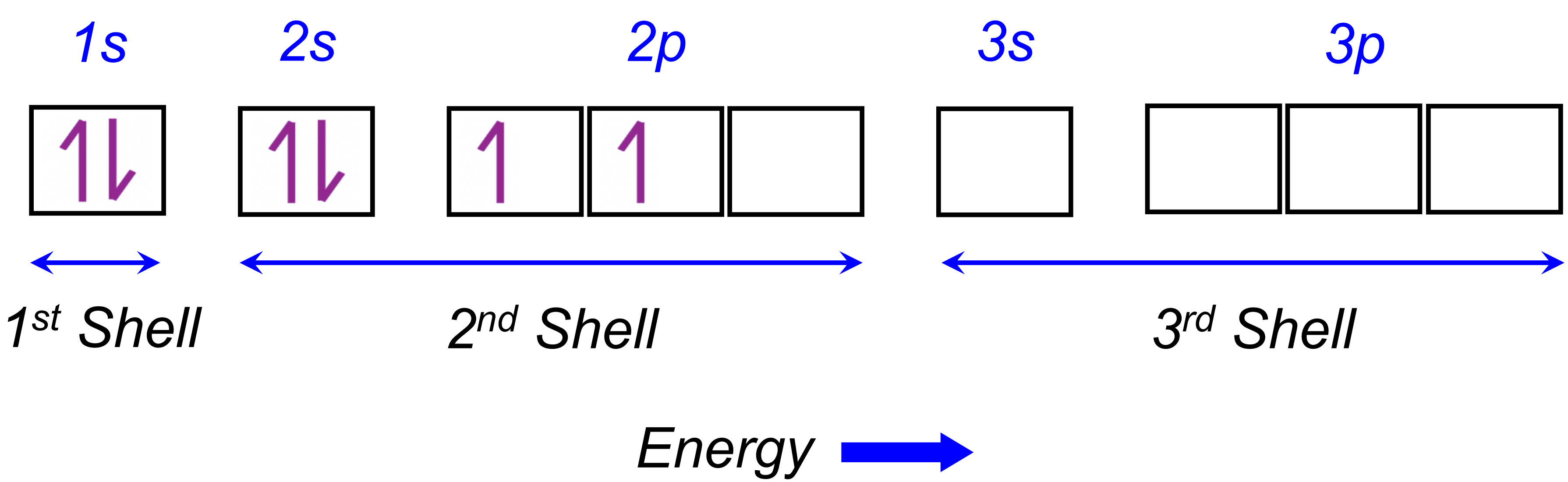
6 – Carbon



Electronic Configurations

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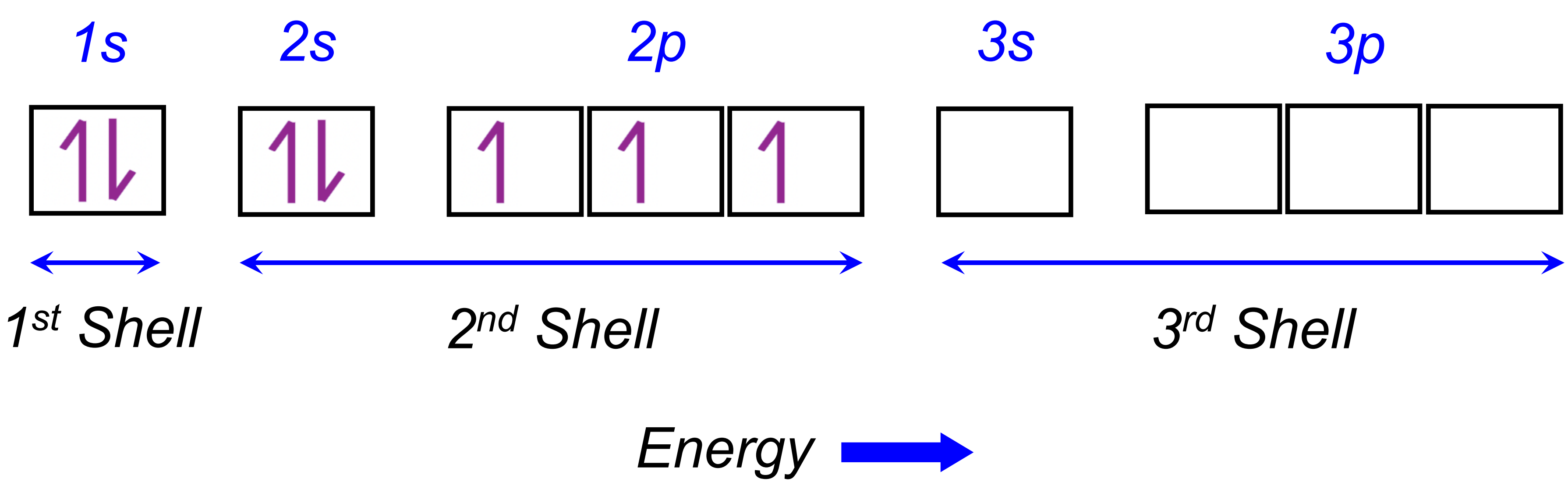
7 – Nitrogen



Electronic Configurations

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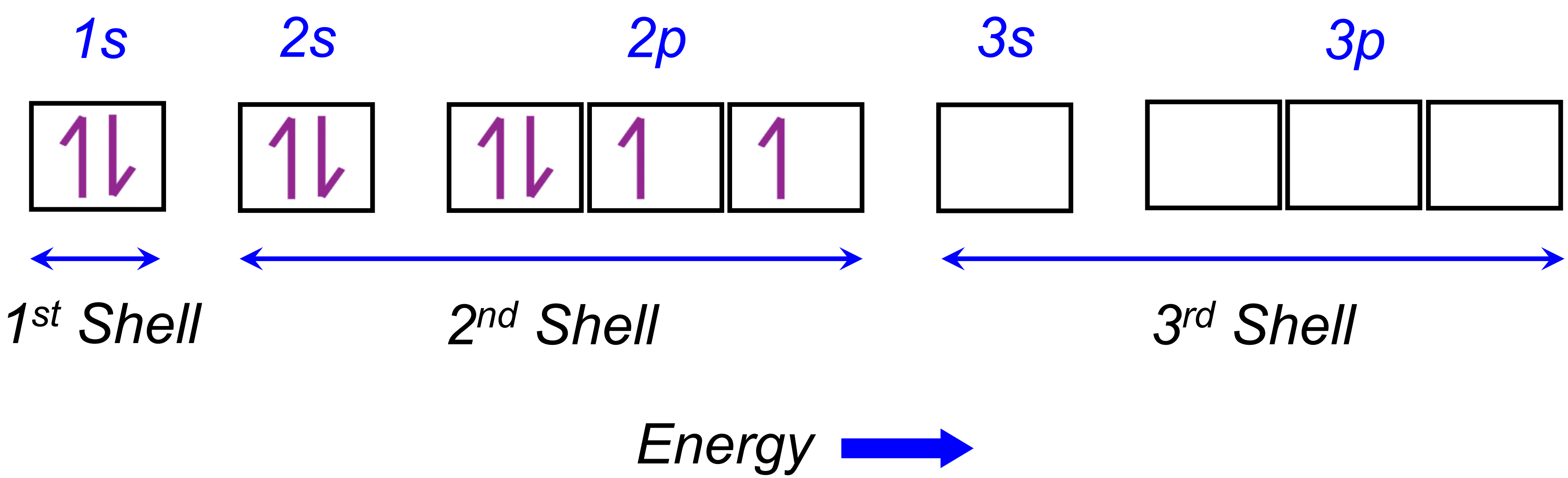
8 – Oxygen



Electronic Configurations

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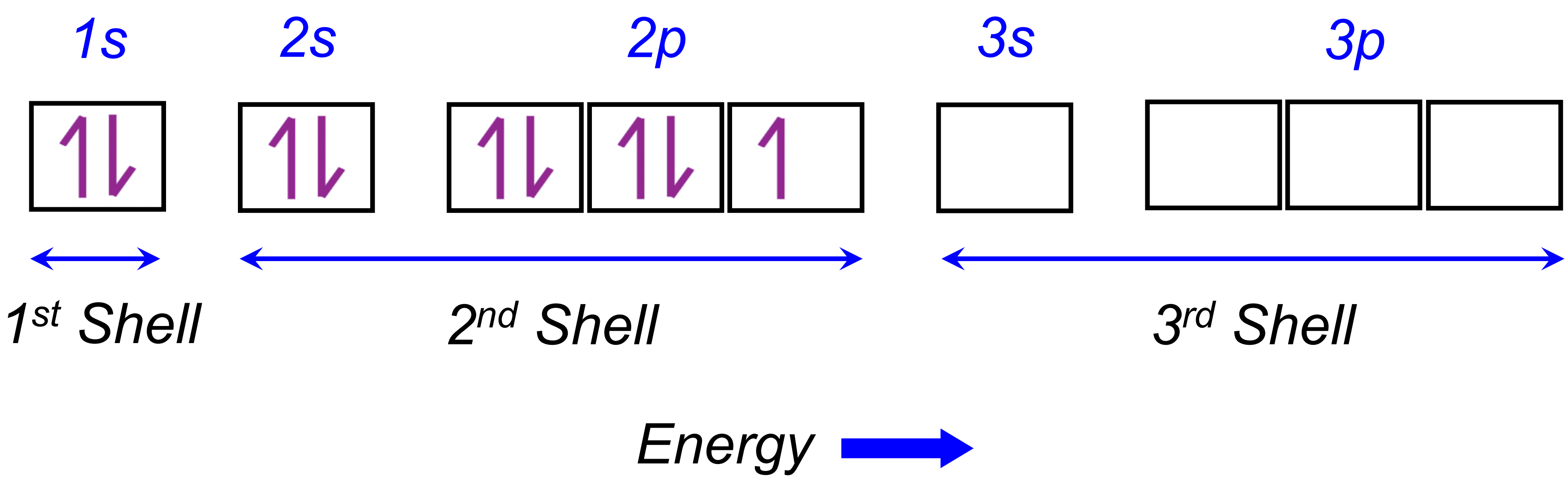
9 – Fluorine



Electronic Configurations

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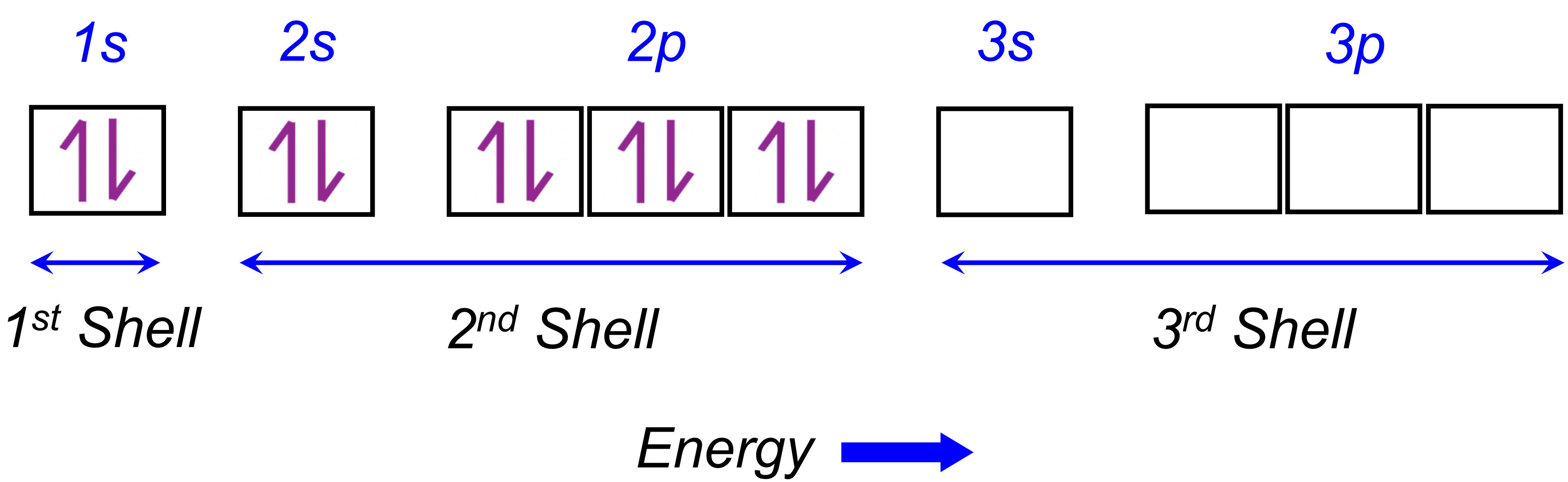
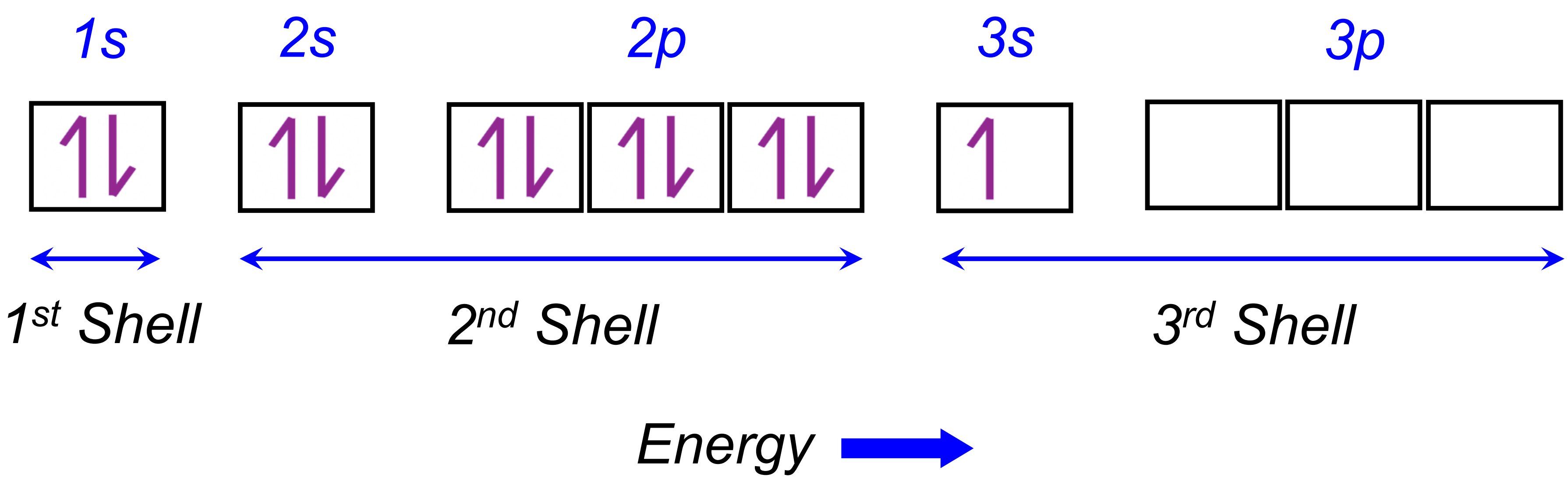
10 – Neon



Electronic Configurations

• Note: Because electrons all carry a charge of –1, they naturally repel each other. Because of this, when electrons enter p-orbitals, they will initially occupy separate p-orbitals before they are forced to pair-up (*spin-pair*) with each other.

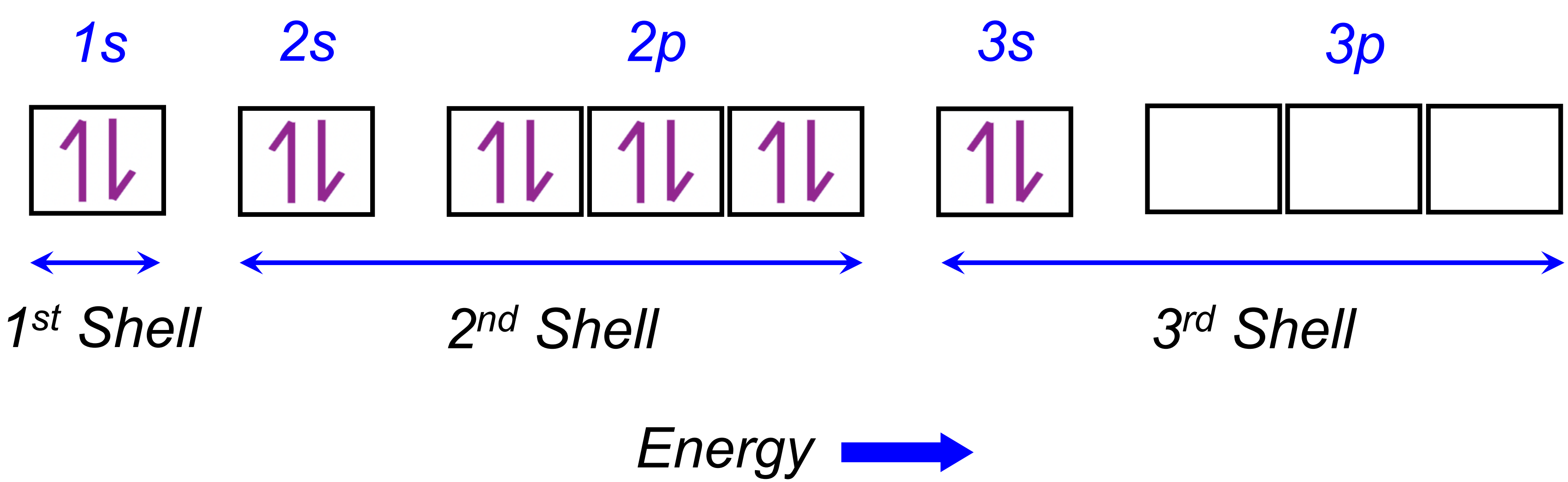
11 – Sodium



Electronic Configurations

• Note: Because electrons all carry a charge of –1, they naturally repel each other. Because of this, when electrons enter p-orbitals, they will initially occupy separate p-orbitals before they are forced to pair-up (*spin-pair*) with each other.

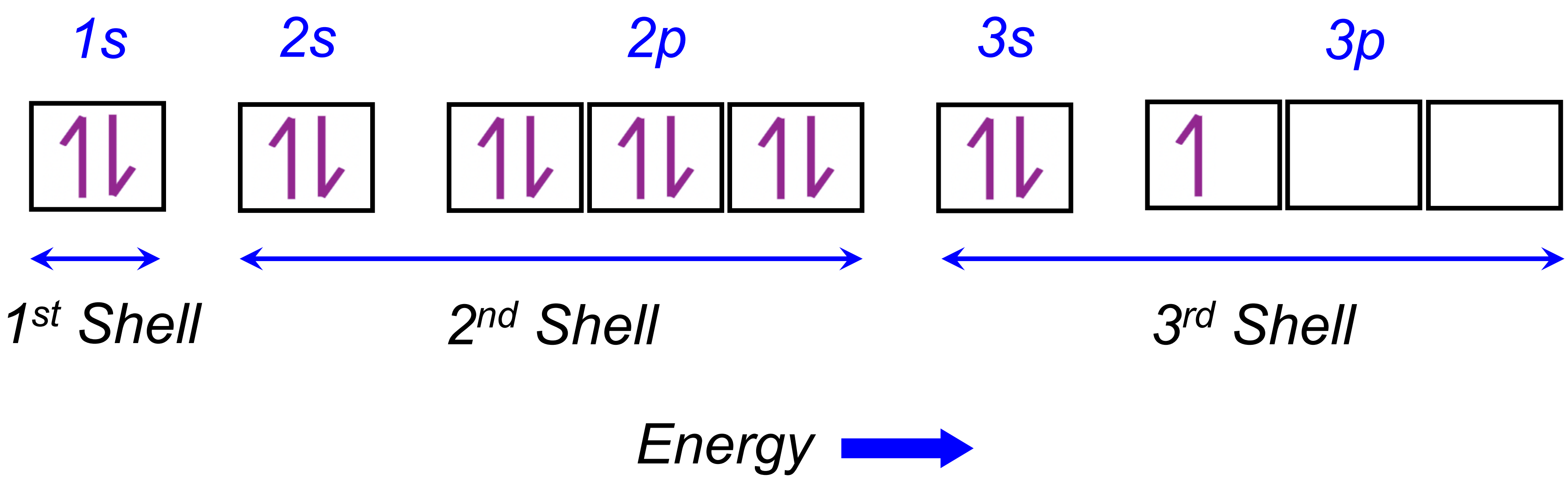
12 – Magnesium



Electronic Configurations

• Note: Because electrons all carry a charge of –1, they naturally repel each other. Because of this, when electrons enter p-orbitals, they will initially occupy separate p-orbitals before they are forced to pair-up (*spin-pair*) with each other.

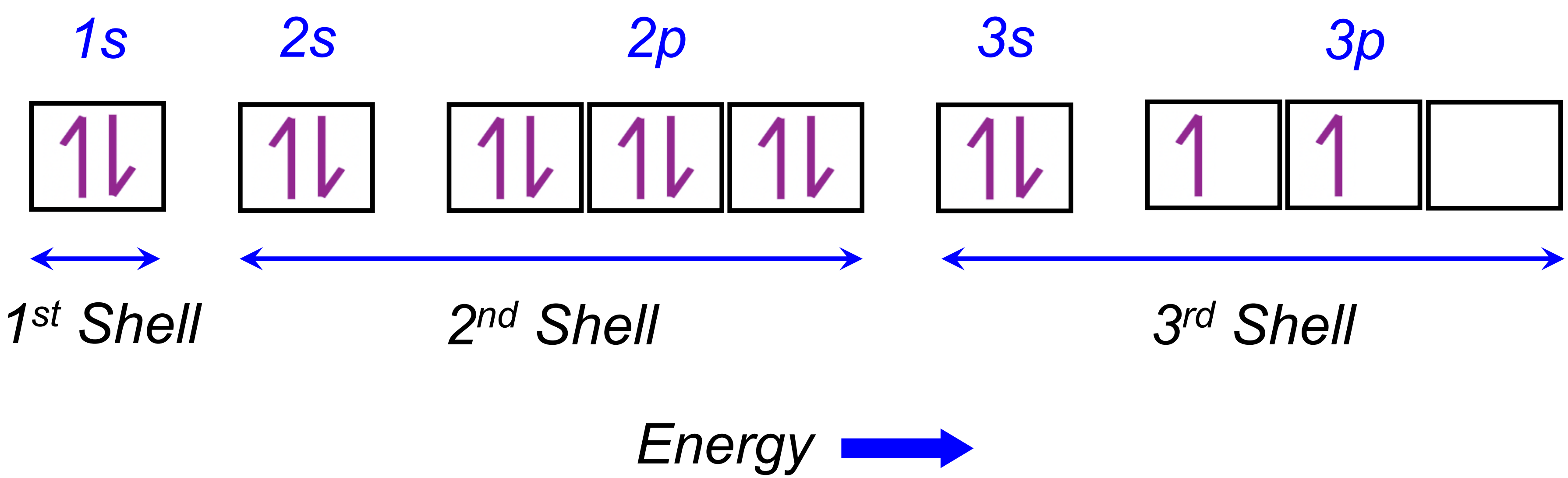
13 – Aluminium



Electronic Configurations

- Note: Because electrons all carry a charge of –1, they naturally repel each other. Because of this, when electrons enter p-orbitals, they will initially occupy separate p-orbitals before they are forced to pair-up (*spin-pair*) with each other.

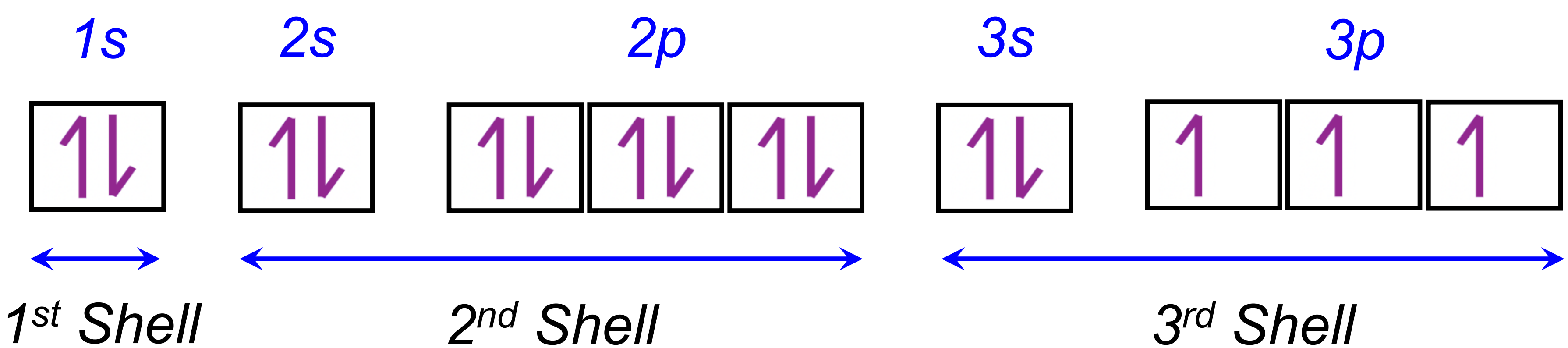
14 – Silicon



Electronic Configurations

- **Note**: Because electrons all carry a charge of –1, they naturally repel each other. Because of this, when electrons enter p-orbitals, they will initially occupy separate p-orbitals before they are forced to pair-up (*spin-pair*) with each other.

15 – Phosphorus

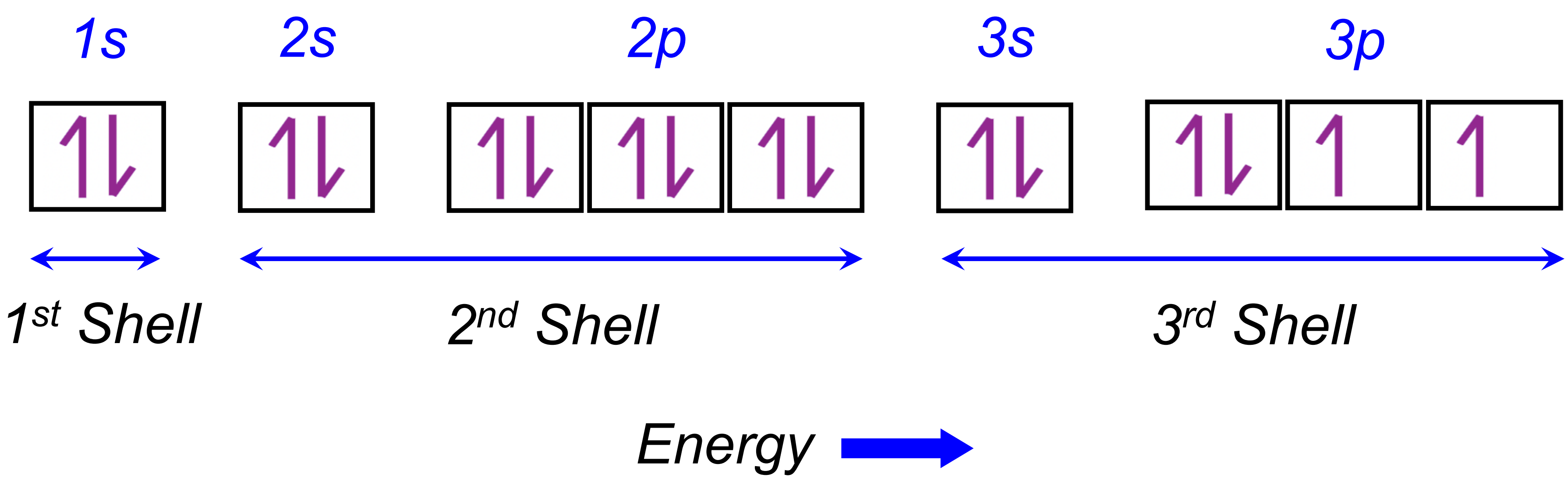


Energy →

Electronic Configurations

• **Note**: Because electrons all carry a charge of –1, they naturally repel each other. Because of this, when electrons enter p-orbitals, they will initially occupy separate p-orbitals before they are forced to pair-up (*spin-pair*) with each other.

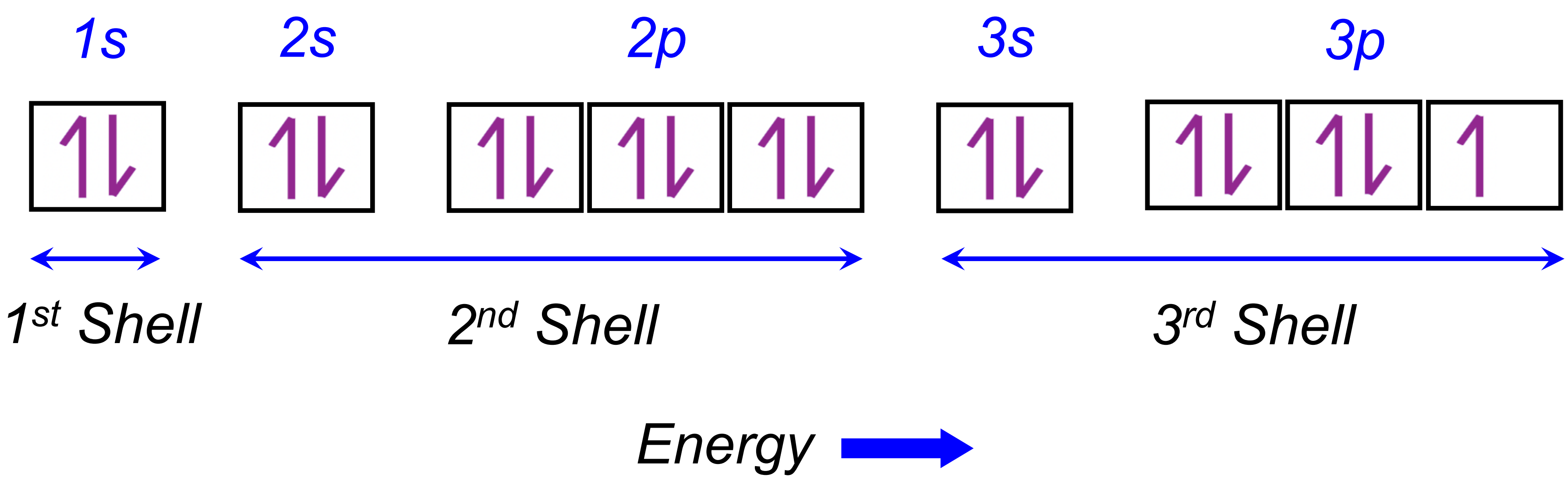
16 – Sulfur



Electronic Configurations

• Note: Because electrons all carry a charge of –1, they naturally repel each other. Because of this, when electrons enter p-orbitals, they will initially occupy separate p-orbitals before they are forced to pair-up (*spin-pair*) with each other.

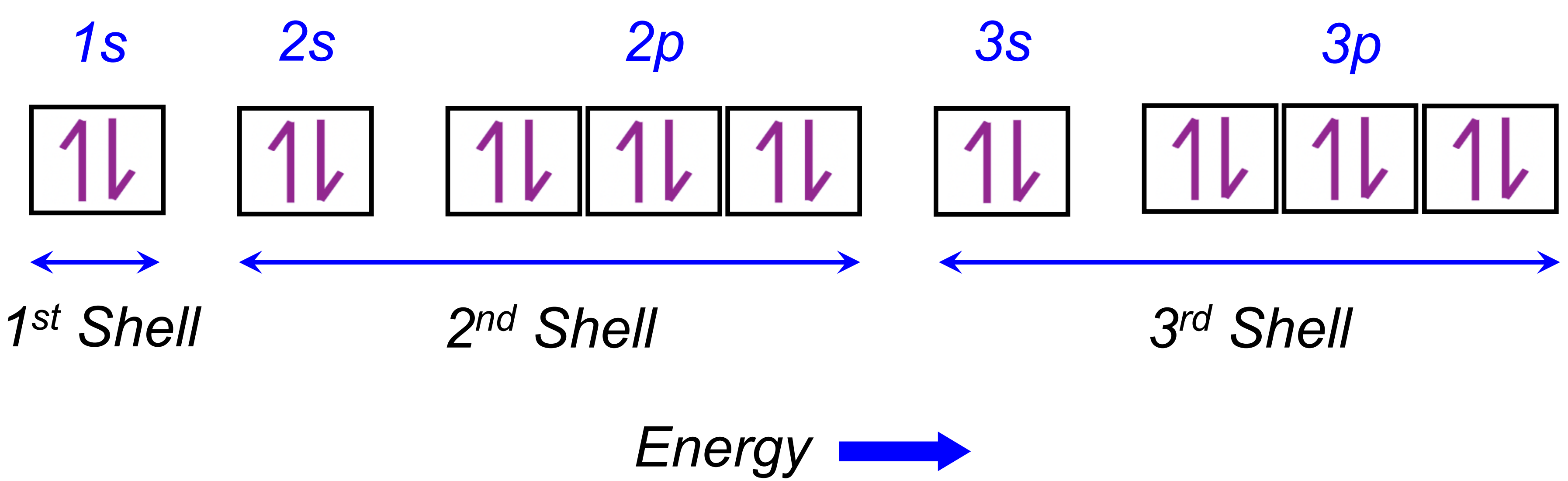
17 – Chlorine



Electronic Configurations

- Note: Because electrons all carry a charge of –1, they naturally repel each other. Because of this, when electrons enter p-orbitals, they will initially occupy separate p-orbitals before they are forced to pair-up (*spin-pair*) with each other.

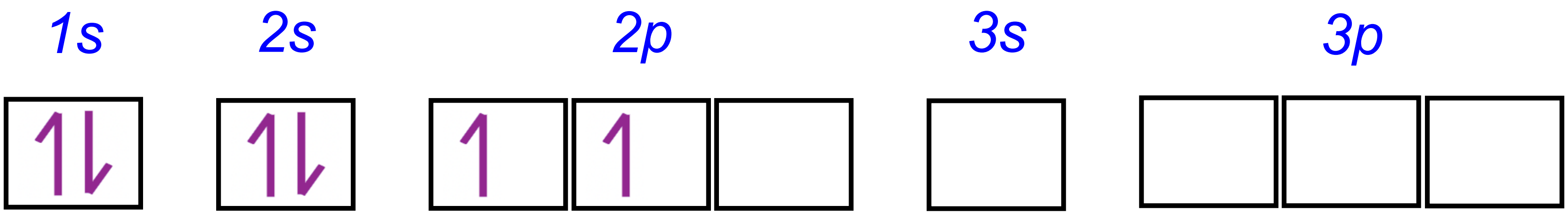
18 – Argon



Electronic Configurations

- The electron configuration of carbon is given below:

Carbon

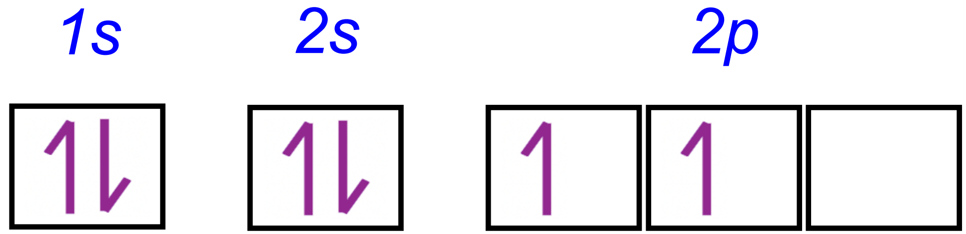


Questions:

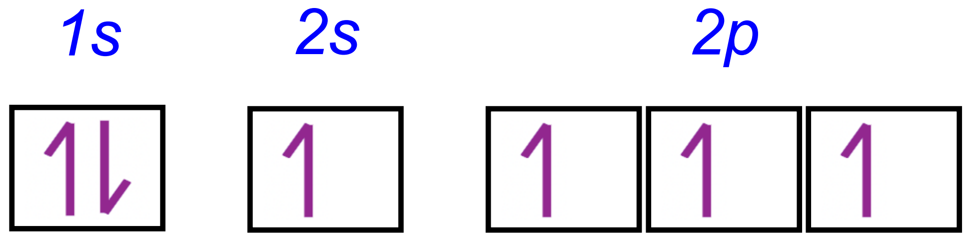
- From the electron configuration shown above, how many covalent bonds would you expect a carbon atom to make?
- How is it possible for a carbon atom to make *four* covalent bonds?

Sp^3 Hybridisation

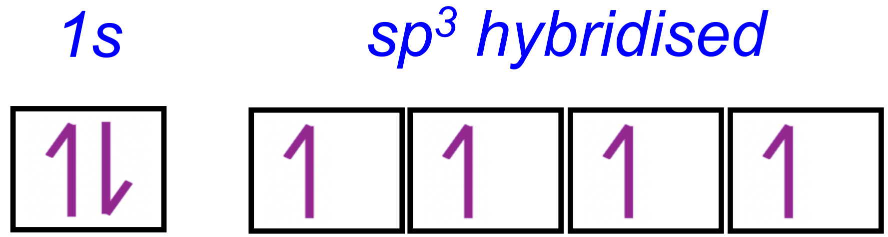
- Carbon (*ground state*):



- Carbon (*excited*):

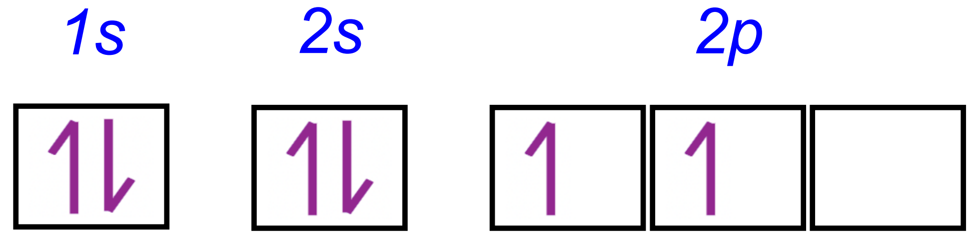


- Carbon (*sp^3 hybridised*):

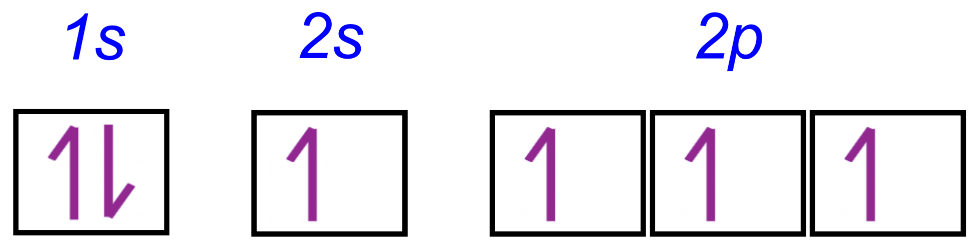


Sp^3 Hybridisation

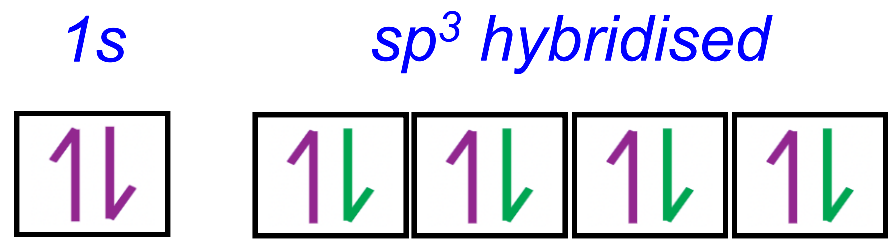
- Carbon (*ground state*):



- Carbon (*excited*):



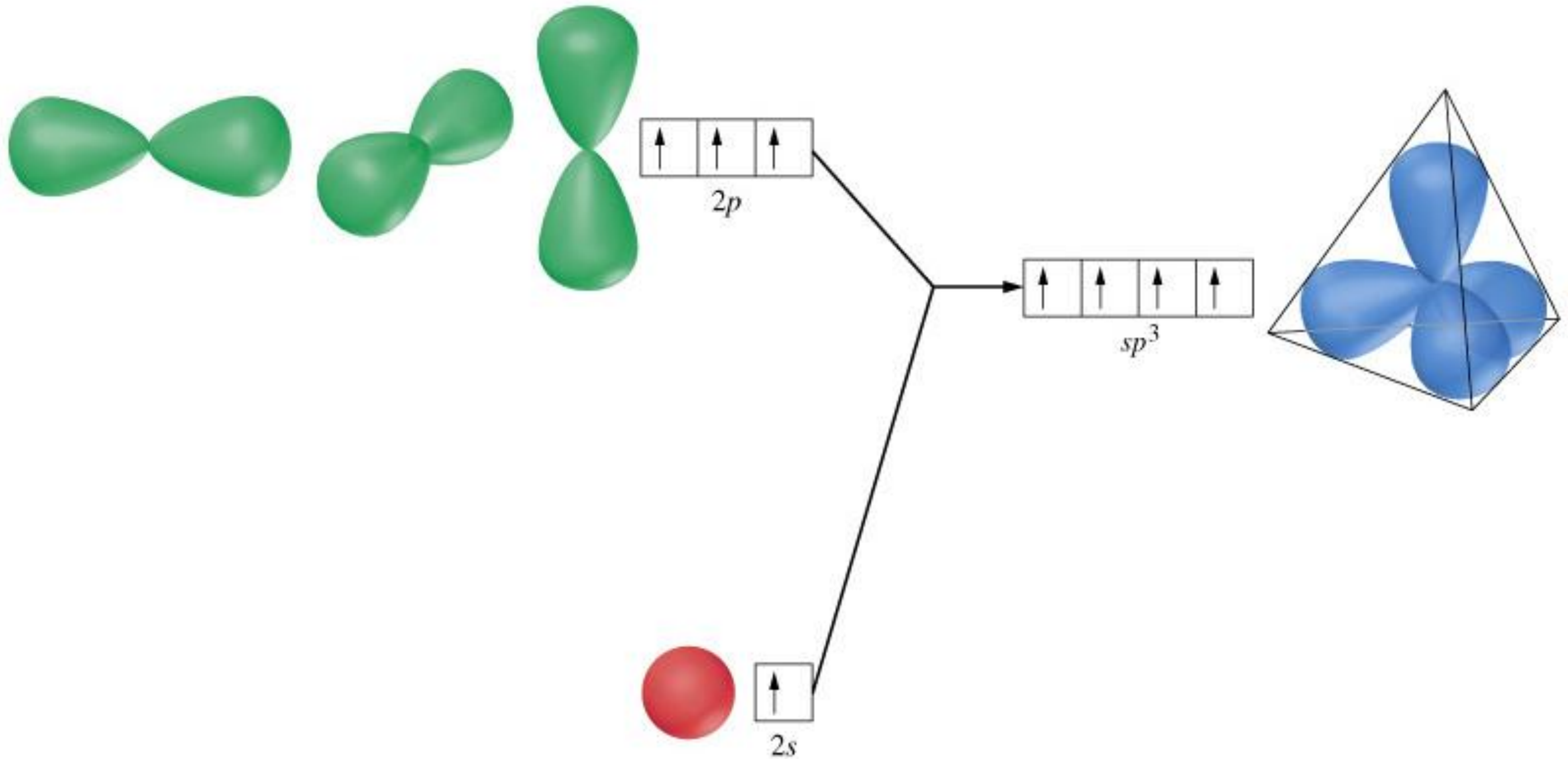
- Carbon (*sp^3 hybridised*):



- Carbon makes *four* covalent bonds.

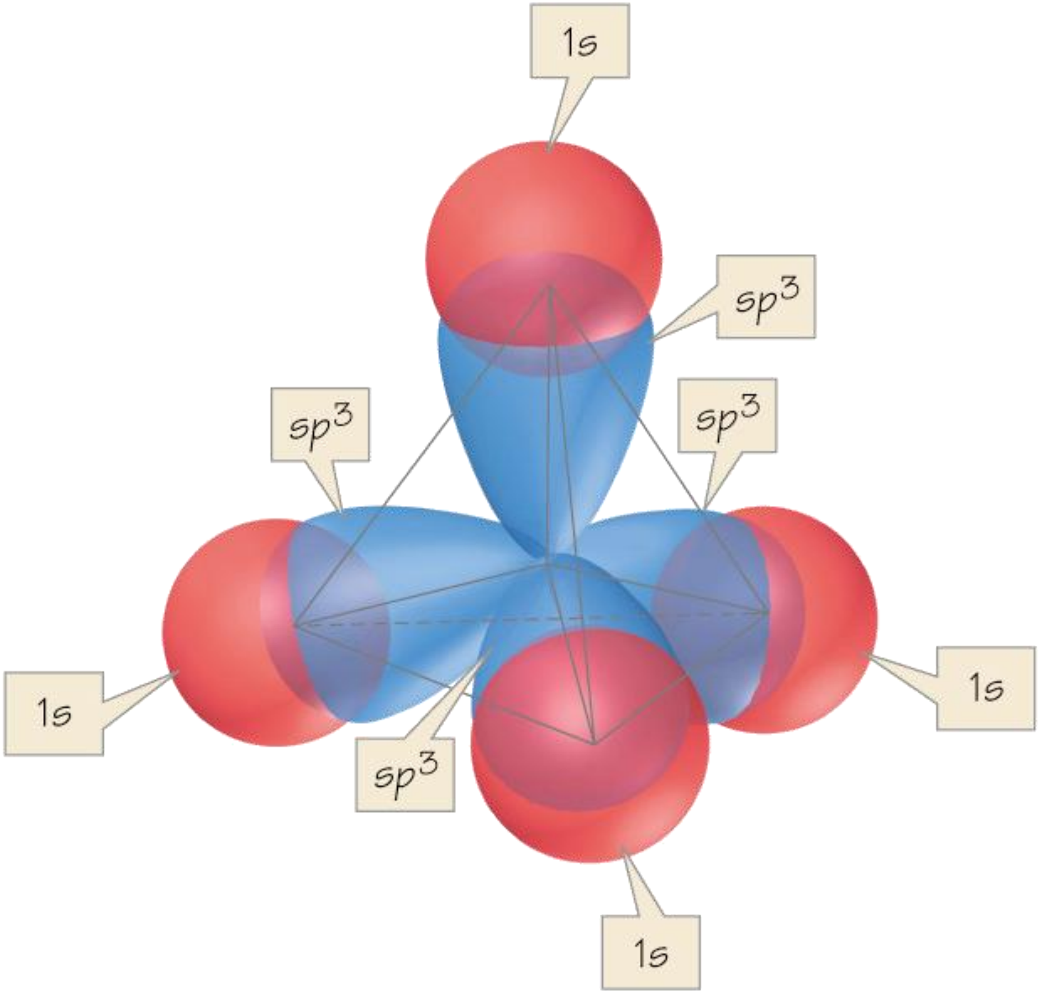
- Key: ↿ = electron of carbon ⇂ = electron of another chemical element.

Sp^3 Hybridisation



- The sp^3 hybridisation of carbon.

Sp^3 Hybridisation

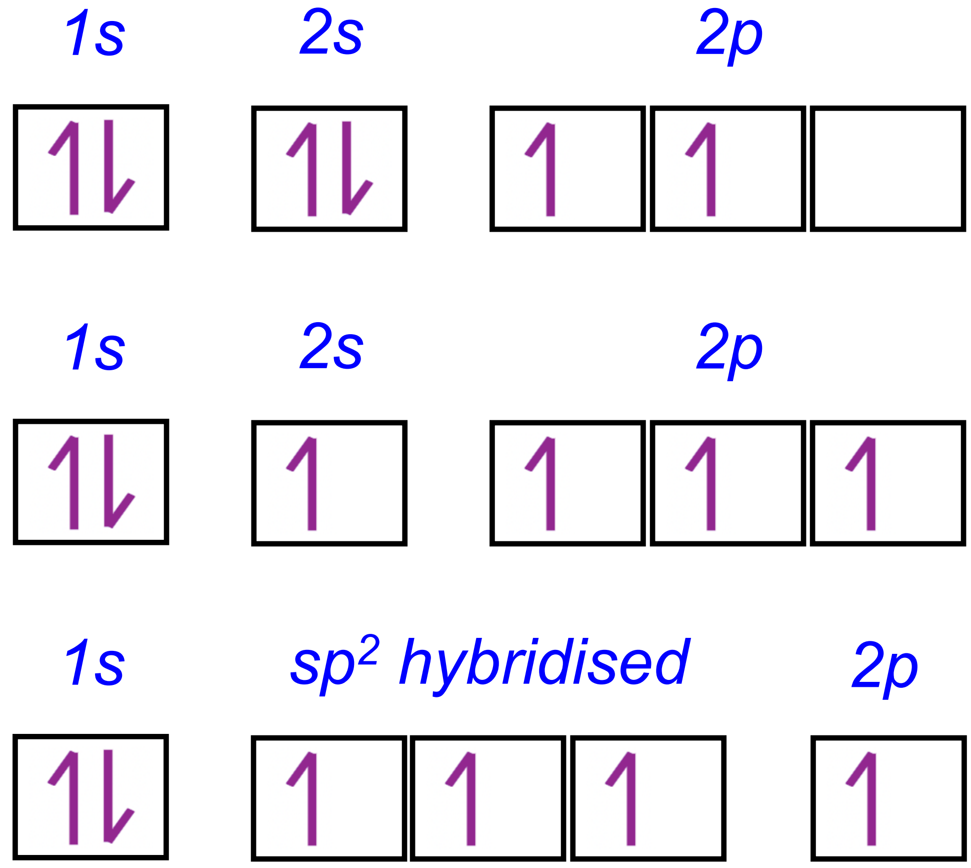


- The bonding in methane (CH_4).

- The four *sp³ hybridised orbitals* of the carbon atom (blue) overlap with the *s-orbitals* of four hydrogen atoms (red) to form four *σ-bonds*.

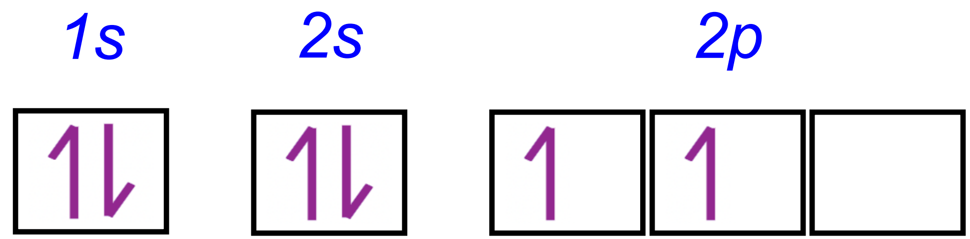
Sp^2 Hybridisation

- Carbon (*ground state*):
- Carbon (*excited*):
- Carbon (*sp^2 hybridised*):

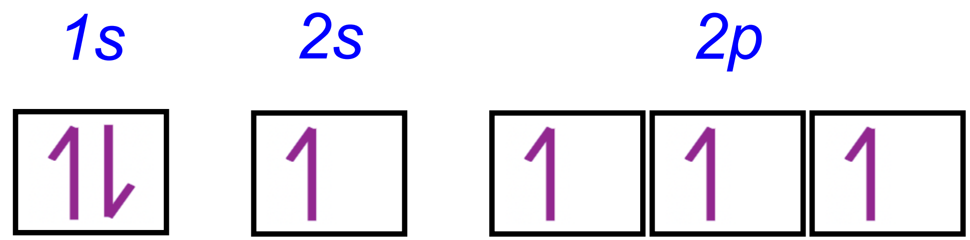


Sp^2 Hybridisation

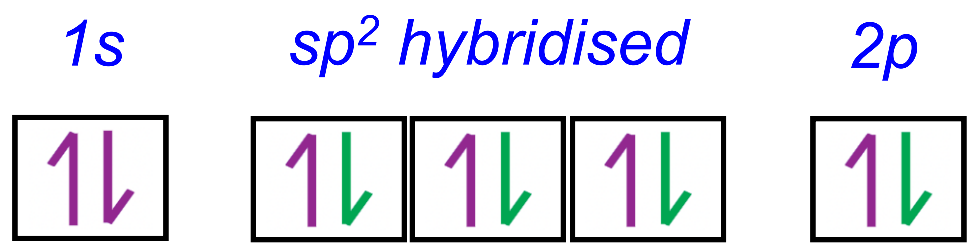
- Carbon (*ground state*):



- Carbon (*excited*):



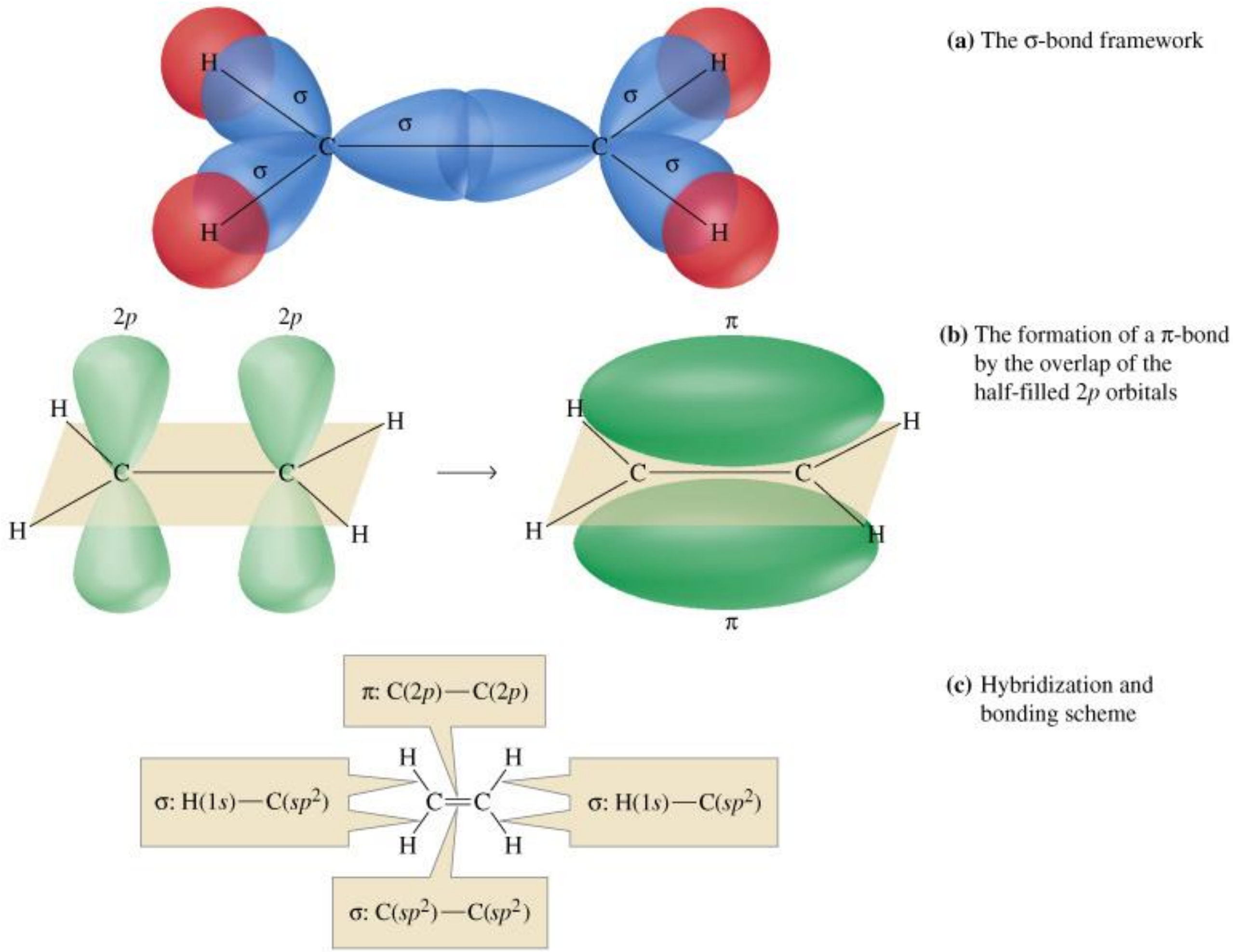
- Carbon (*sp^2 hybridised*):



- Carbon makes *four* covalent bonds.

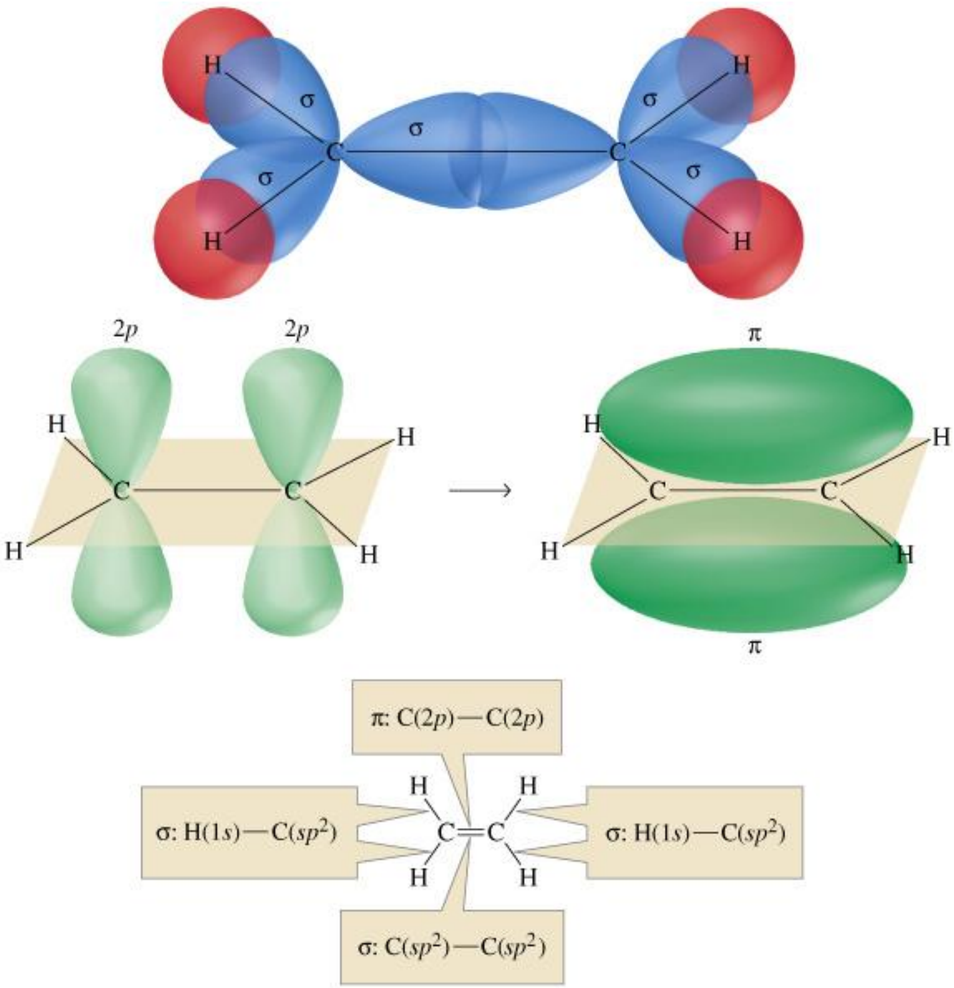
- Key:  = electron of carbon  = electron of another chemical element.

Sp^2 Hybridisation



- The bonding in ethene (C_2H_4) *#1*.
- The three *sp^2 hybridised orbitals* of each carbon atom (blue) overlap with each other and also with the *s-orbitals* of four hydrogen atoms (red) to form a total of five *σ-bonds*.

Sp^2 Hybridisation



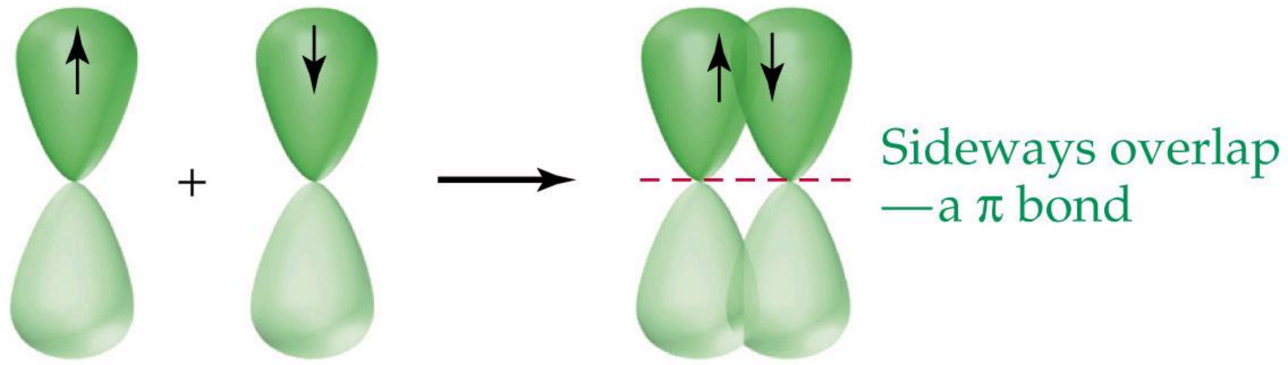
(a) The σ-bond framework

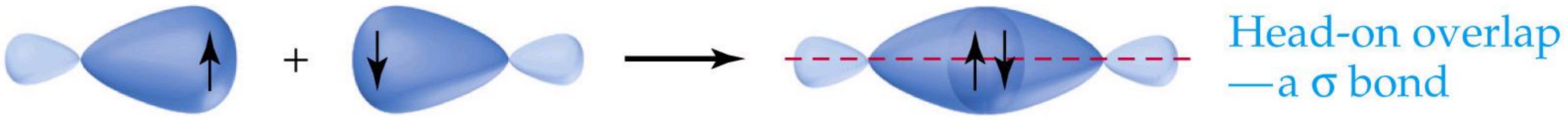
(b) The formation of a π-bond by the overlap of the half-filled 2*p* orbitals

(c) Hybridization and bonding scheme

- The bonding in ethene (C_2H_4) #2.
- The *p-orbitals* of each carbon atom which are not hybridised (green) are arranged parallel to each other. They overlap above and below the plane of the molecule forming a *π-bond*.

σ-Bonds and π-Bonds





- A comparison of *σ-bonds* and *π-bonds*:

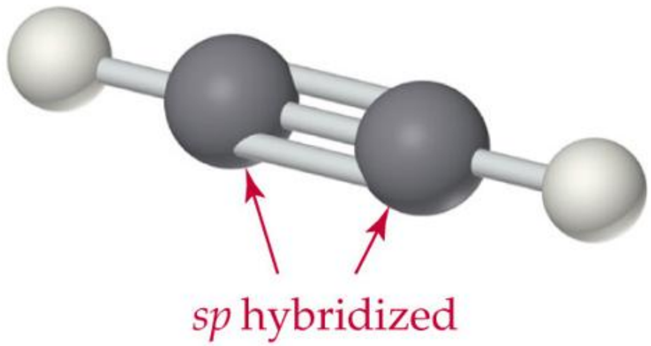
- *σ-bonds* are formed when the region of orbital overlap lies directly between the nuclei of the two bonding atoms.

- *π-bonds* are formed when the region of orbital overlap does not lie directly between the nuclei of the two bonding atoms, but instead lies above and below the plane of the molecule.

The Existence of C$\equiv$C Bonds

Question:

- Elaborate on this information to propose a model for the bonding in *ethyne*:

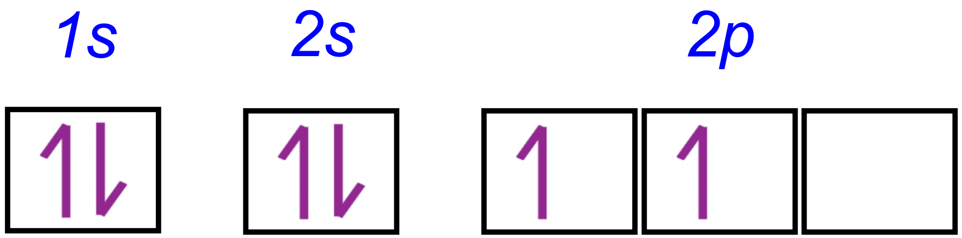


Your answer should take into account:

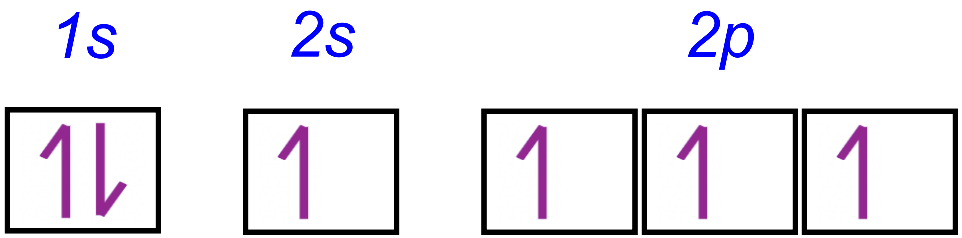
→ The existence of *s-orbitals* and *p-orbitals*.
→ The ability for carbon's *2s* and *2p* orbitals to *hybridise*.
→ The *linear* shape of the ethyne molecule.

Sp Hybridisation

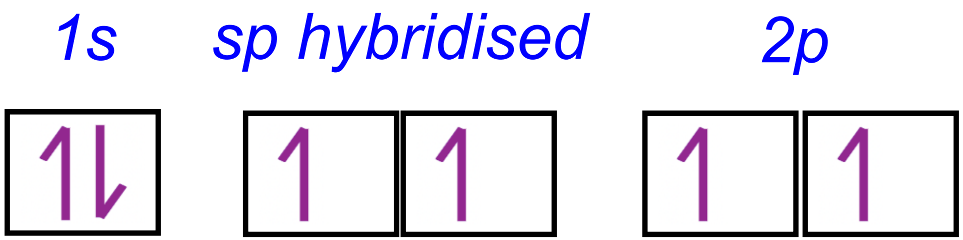
- Carbon (*ground state*):



- Carbon (*excited*):

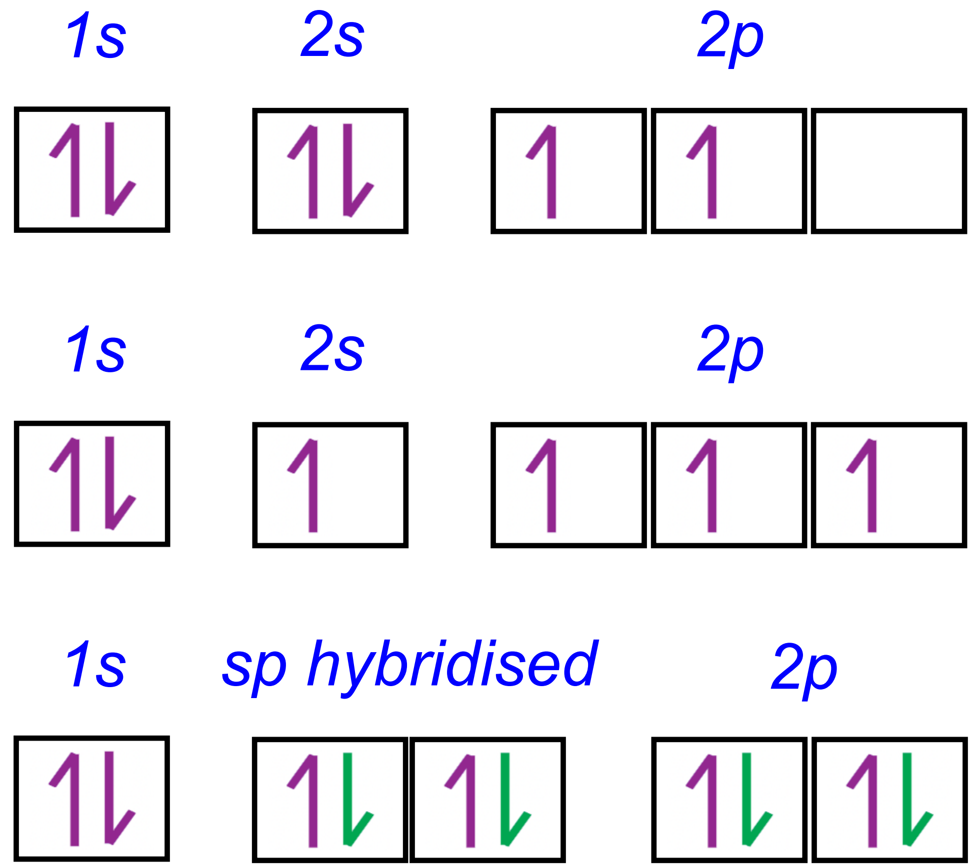


- Carbon (*sp hybridised*):



Sp Hybridisation

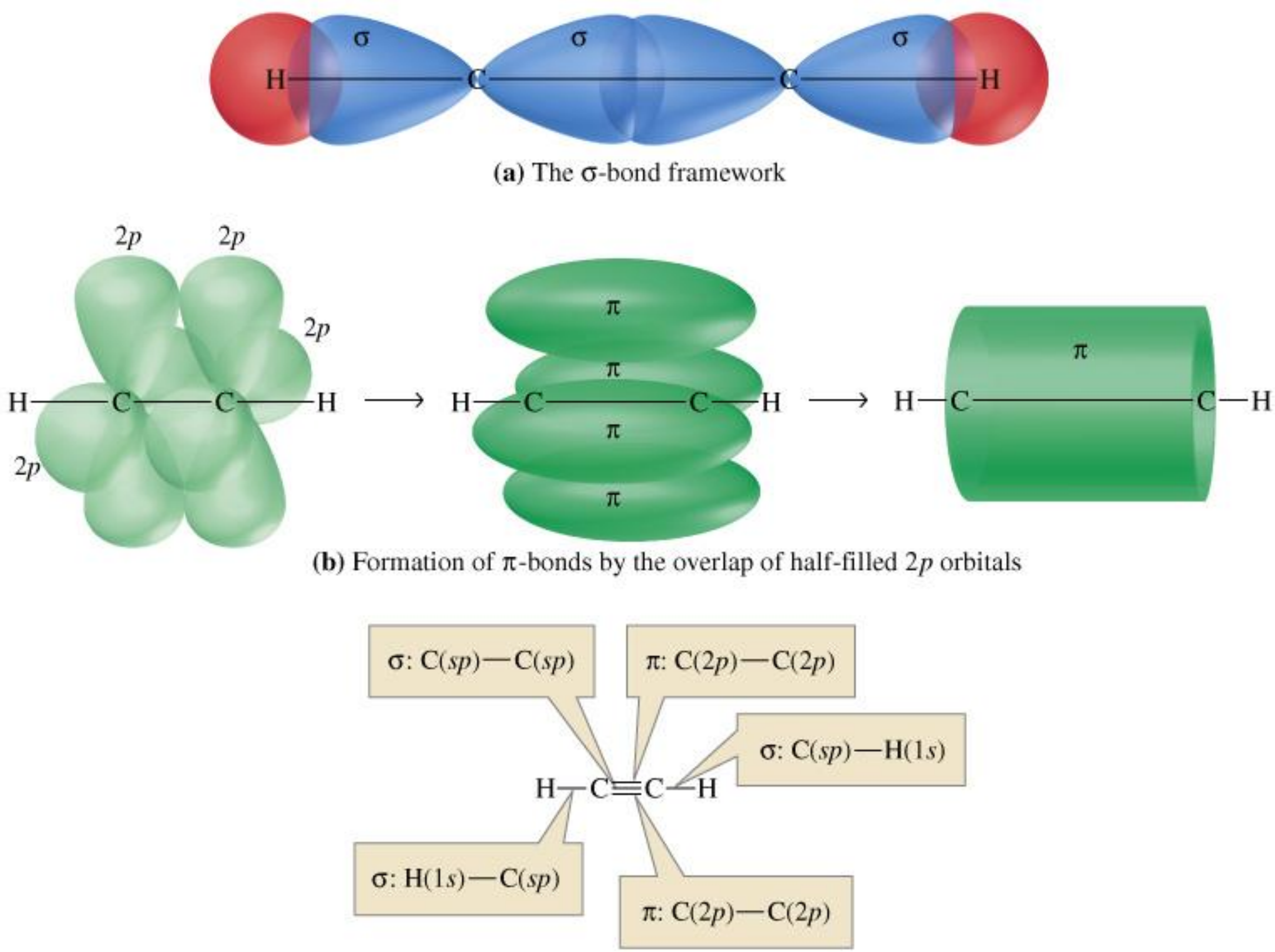
- Carbon (*ground state*):
- Carbon (*excited*):
- Carbon (*sp hybridised*):



- Carbon makes *four* covalent bonds.

- Key: ↿ = electron of carbon ⇂ = electron of another chemical element.

Sp Hybridisation



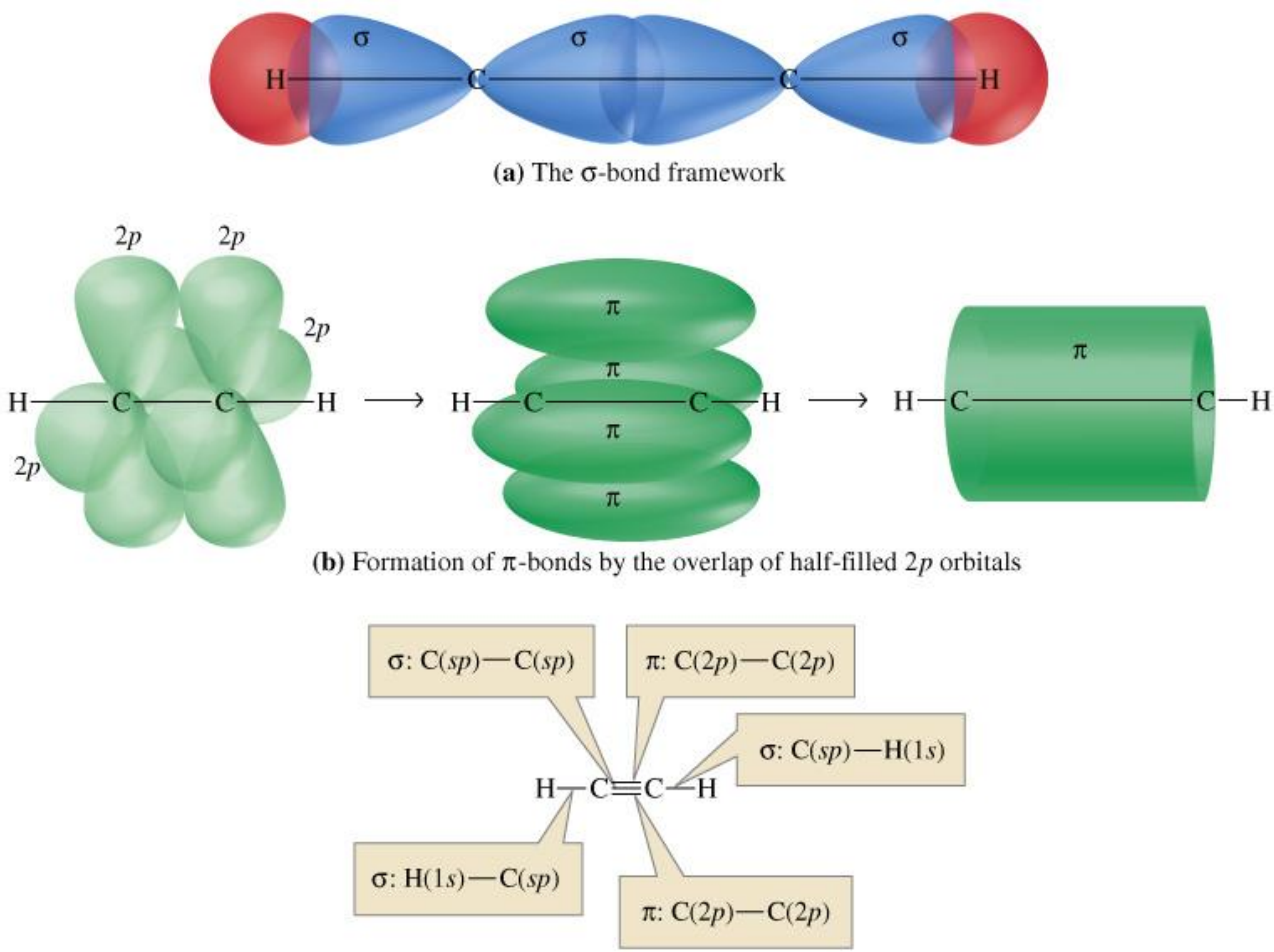
(a) The σ-bond framework

(b) Formation of π-bonds by the overlap of half-filled 2p orbitals

(c) Hybridization and bonding scheme

- The bonding in ethyne (C_2H_2) *#1*.
- The *sp hybridised orbitals* of each carbon atom (blue) overlap with each other and also with the *s-orbitals* of two hydrogen atoms (red) to form a total of three *σ-bonds* arranged in a *linear* formation.

Sp Hybridisation



(a) The σ-bond framework

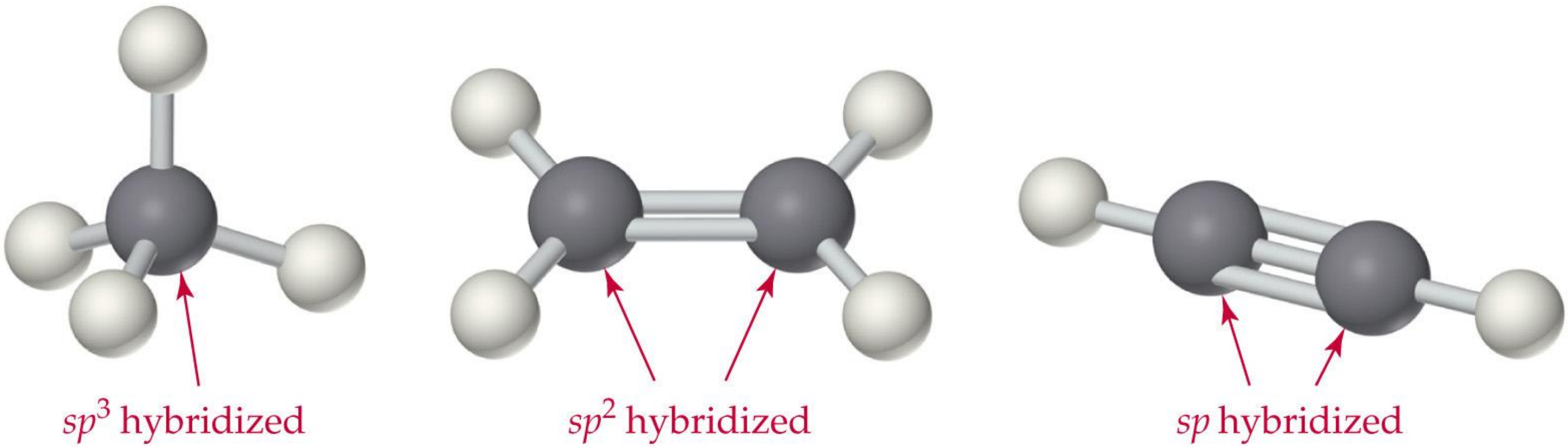
(b) Formation of π-bonds by the overlap of half-filled 2p orbitals

(c) Hybridization and bonding scheme

- The bonding in ethyne (C_2H_2) #2.

- Each carbon atom has *two p-orbitals* (green) which are not hybridised. They arranged at 90° to each other within the same carbon atom and parallel to each other between the individual carbon atoms. Overlap of the four p-orbitals results in the formation of *two π-bonds* between the two carbon atoms.

A Summary of sp^3, sp^2 and sp Hybridisation



- The carbon atoms forming a $C - C$ bond are sp^3 *hybridised*.
- The carbon atoms forming a $C = C$ bond are sp^2 *hybridised*.
- The carbon atoms forming a $C \equiv C$ bond are *sp hybridised*.

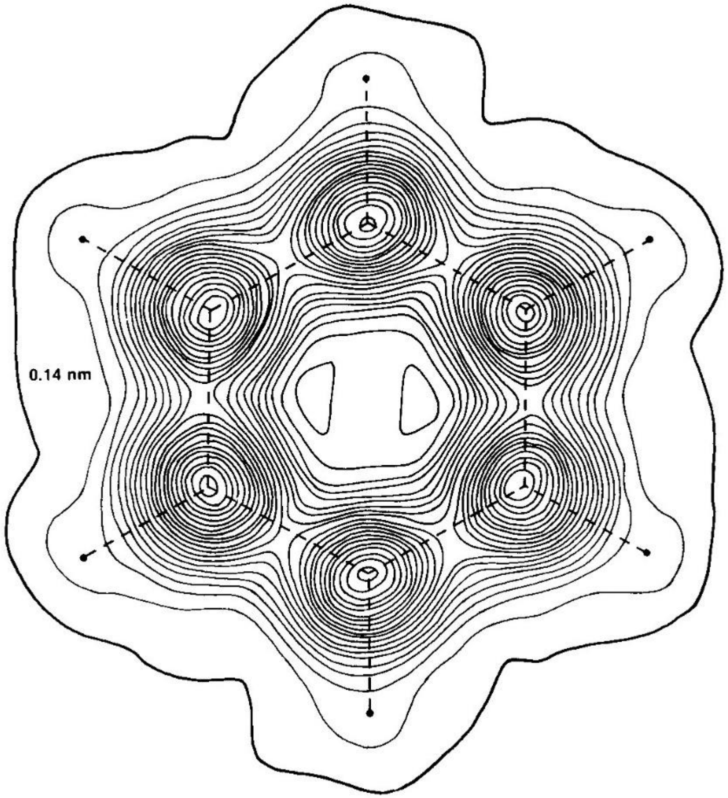
The Modern Structure of Benzene

Question:

- With this information, propose a structure for benzene, formula C_6H_6, which takes into account:

→ The existence of *s-orbitals* and *p-orbitals*.
→ The ability for carbon's *2s* and *2p* orbitals to *hybridise*.
→ The shape of the benzene molecule as determined by *x-ray crystallography*.
→ The relative *stability* of benzene.

The Modern Structure of Benzene



- The structure of benzene (C_6H_6) determined by x-ray crystallography. **Note**: the six carbon atoms are arranged in a planar six-membered ring and all of the carbon-to-carbon covalent bonds are the same length.

The Modern Structure of Benzene

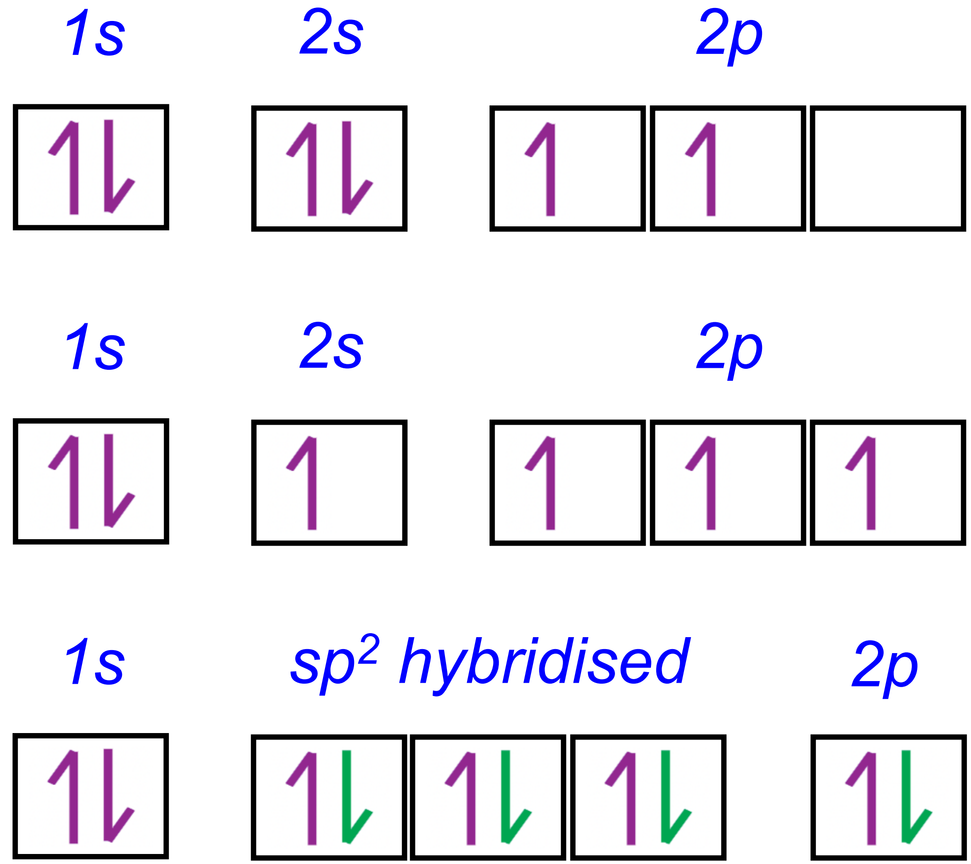
	1s	2s	2p		
• Carbon (*ground state*):	↑↓	↑↓	↑	↑	

	1s	2s	2p		
• Carbon (*excited*):	↑↓	↑	↑	↑	↑

	1s	sp^2 hybridised			2p
• Carbon (*sp^2 hybridised*):	↑↓	↑	↑	↑	↑

The Modern Structure of Benzene

- Carbon (*ground state*):
- Carbon (*excited*):
- Carbon (*sp*^{2} *hybridised*):

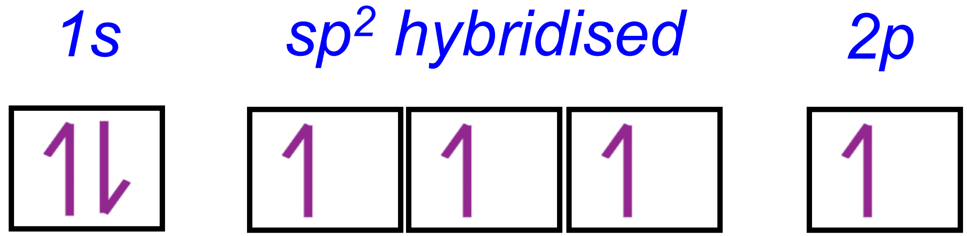


- Carbon makes *four* covalent bonds.

- Key: ↿ = electron of carbon ⇂ = electron of another chemical element.

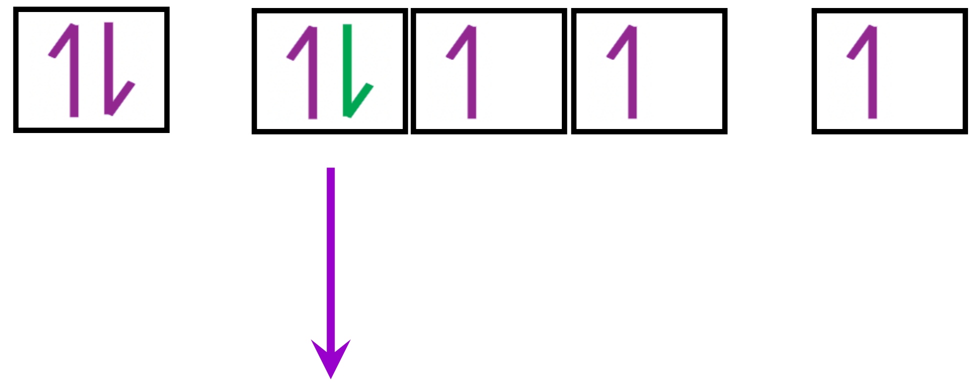
The Modern Structure of Benzene

- Carbon atom in *benzene*:



The Modern Structure of Benzene

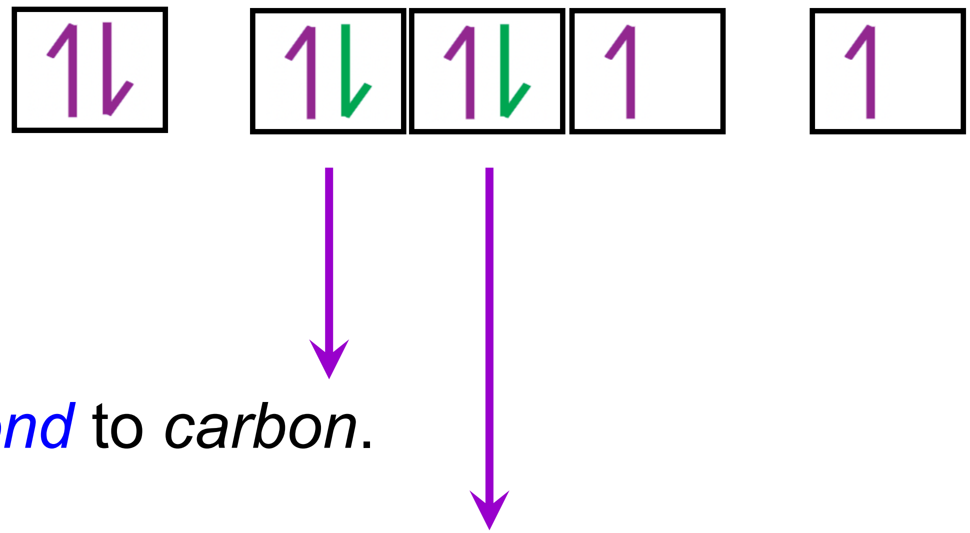
- Carbon atom in *benzene*: *1s* *sp^2 hybridised* *2p*



σ-bond to *carbon*.

The Modern Structure of Benzene

1s *sp^2 hybridised* *2p*

- Carbon atom in *benzene*: 

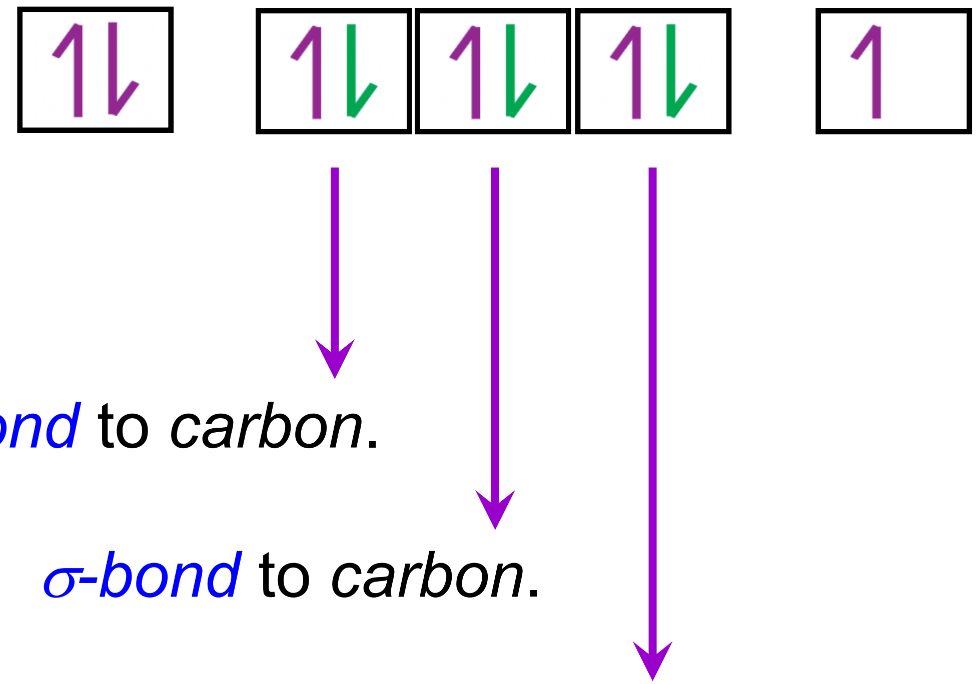
σ-bond to *carbon*.

σ-bond to *carbon*.

The Modern Structure of Benzene

1s — *sp^2 hybridised* — *2p*

- Carbon atom in *benzene*:



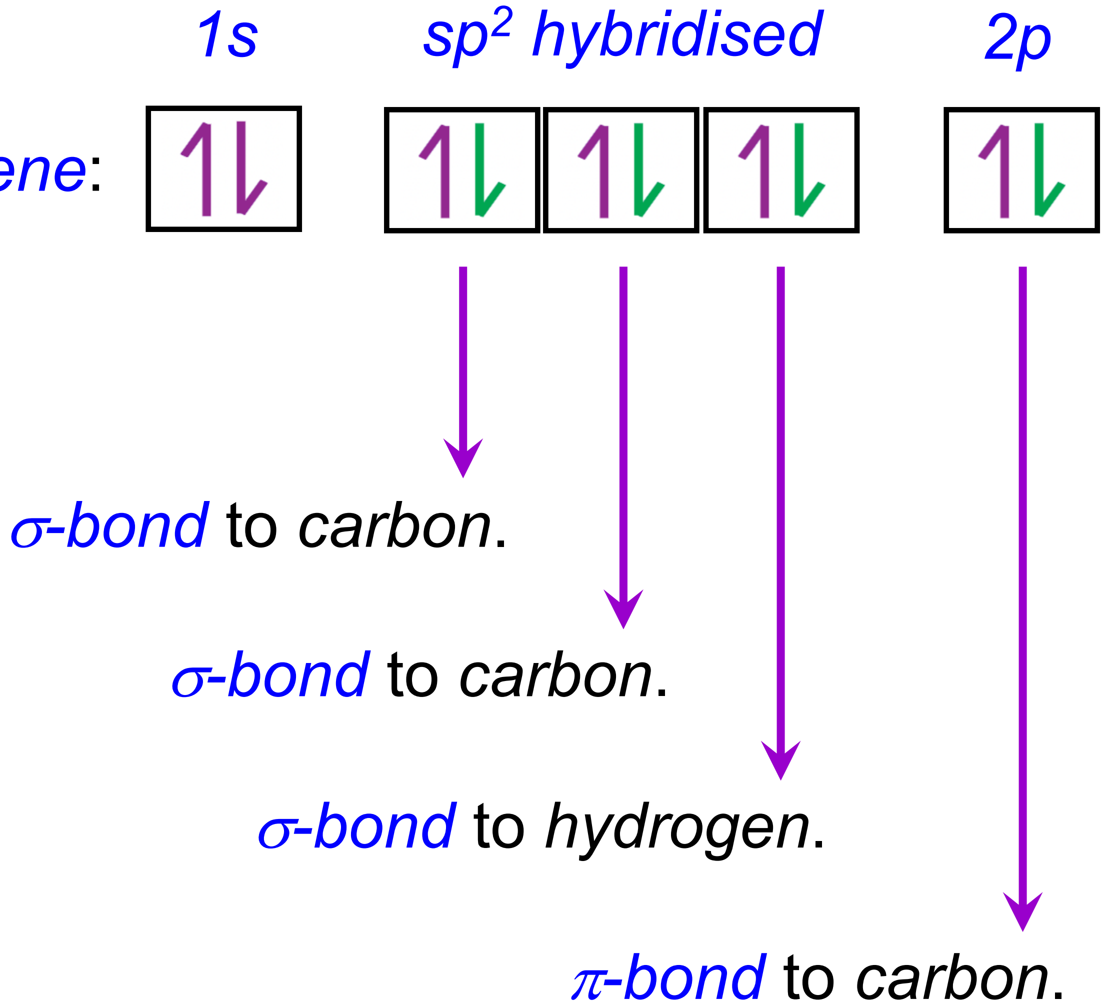
σ-bond to *carbon*.

σ-bond to *carbon*.

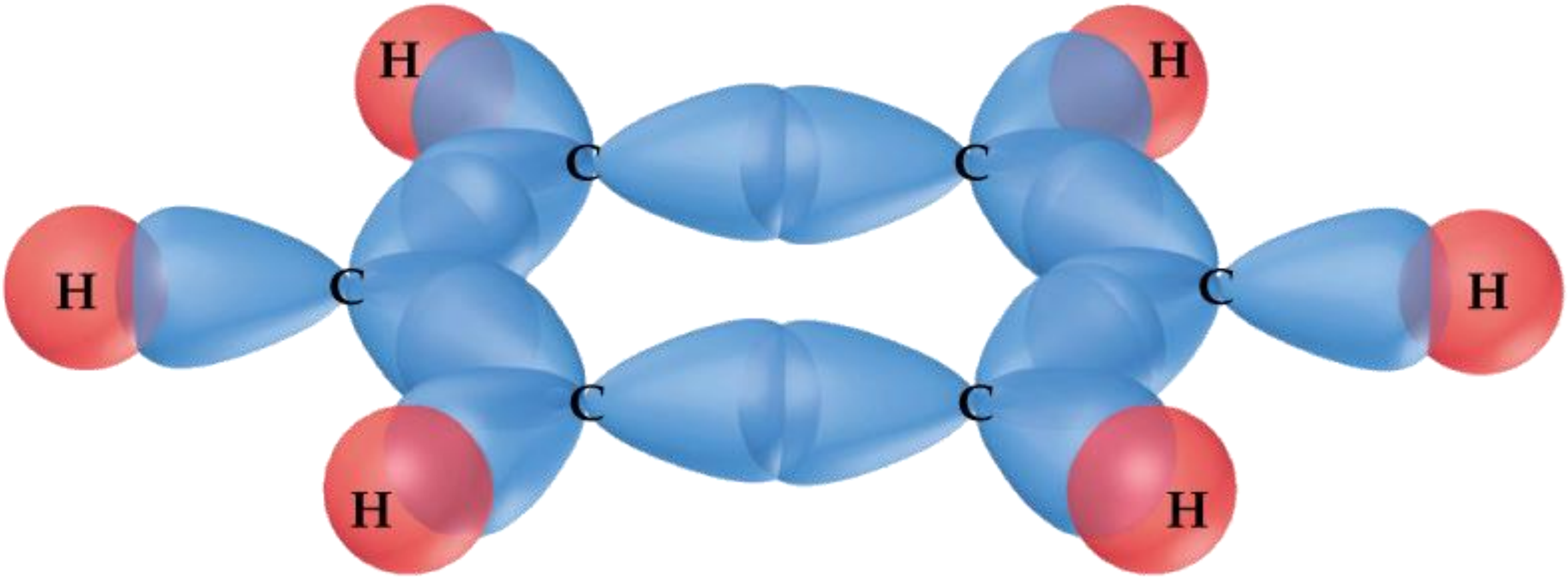
σ-bond to *hydrogen*.

The Modern Structure of Benzene

- Carbon atom in *benzene*:



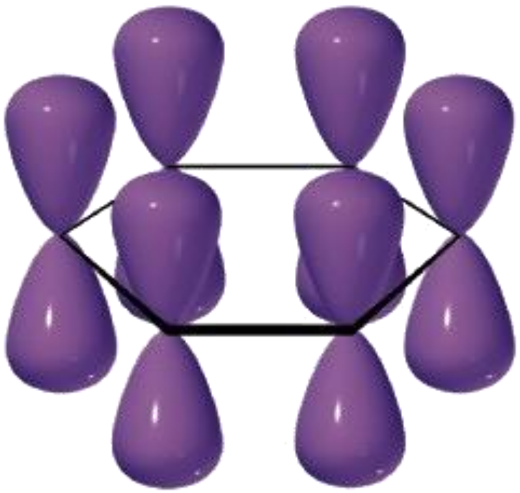
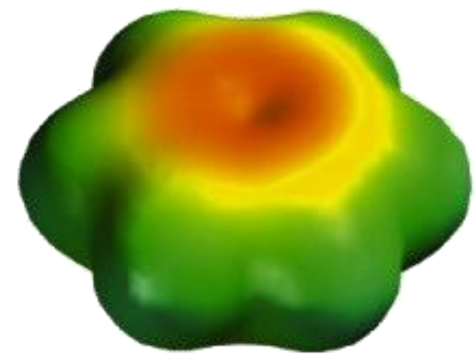
The Modern Structure of Benzene



- The structure of benzene *#1*.

- All six of the carbon atoms in benzene are *sp^2 hybridised*. This results in *σ-bonding* between the sp^2 hybridised orbitals of carbon (blue) and the *s-orbitals* of hydrogen (red).

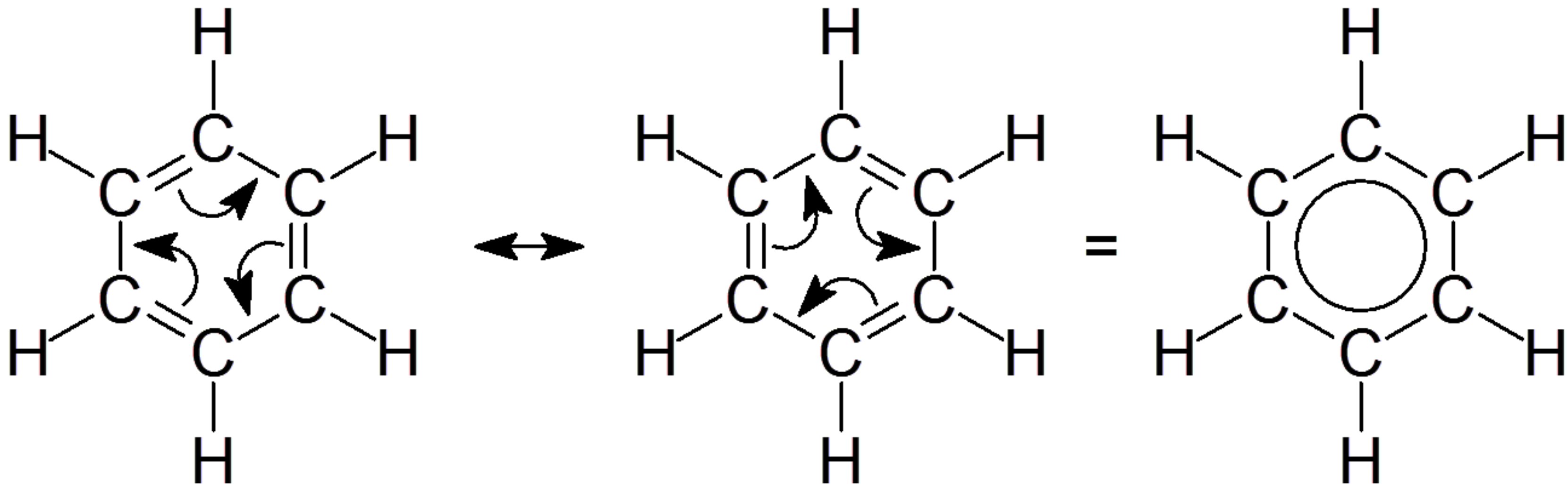
The Modern Structure of Benzene

- The structure of benzene #2.

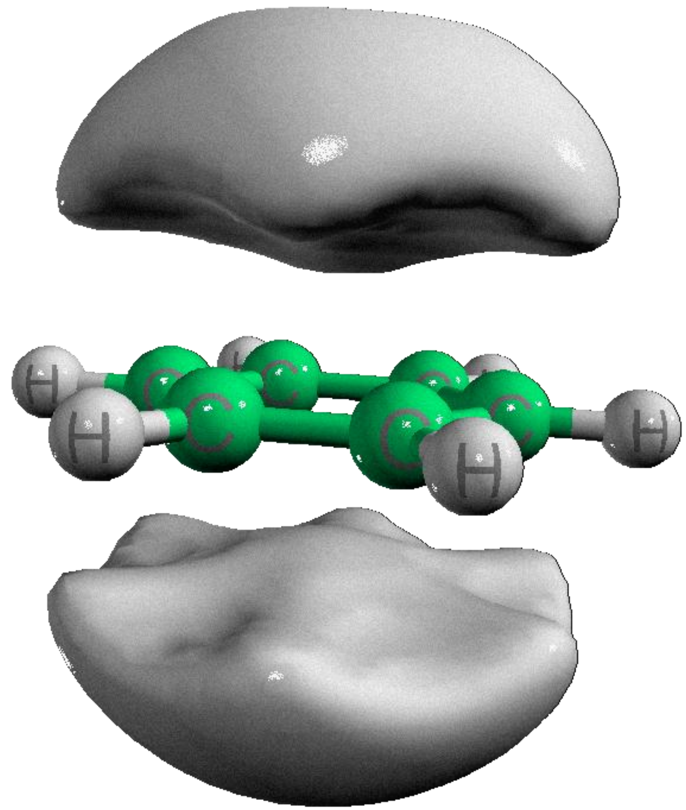
- The *p-orbitals* of carbon which are not hybridised (purple) are arranged parallel to each other and overlap both above and below the plane of the benzene ring forming a cloud of *delocalised of π-bonding electrons*.

The Modern Structure of Benzene



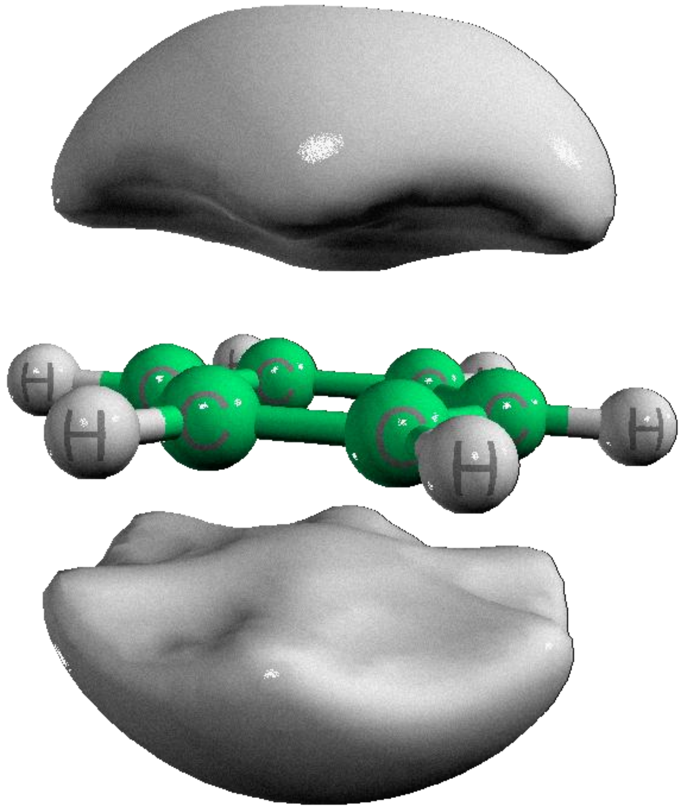
- *Delocalisation* of the *π-bonding electrons* around the benzene ring lowers the energy of the structure by approximately *150 kJ mol*$^{-1}$, a value often referred to as the *delocalisation enthalpy*.

The Modern Structure of Benzene

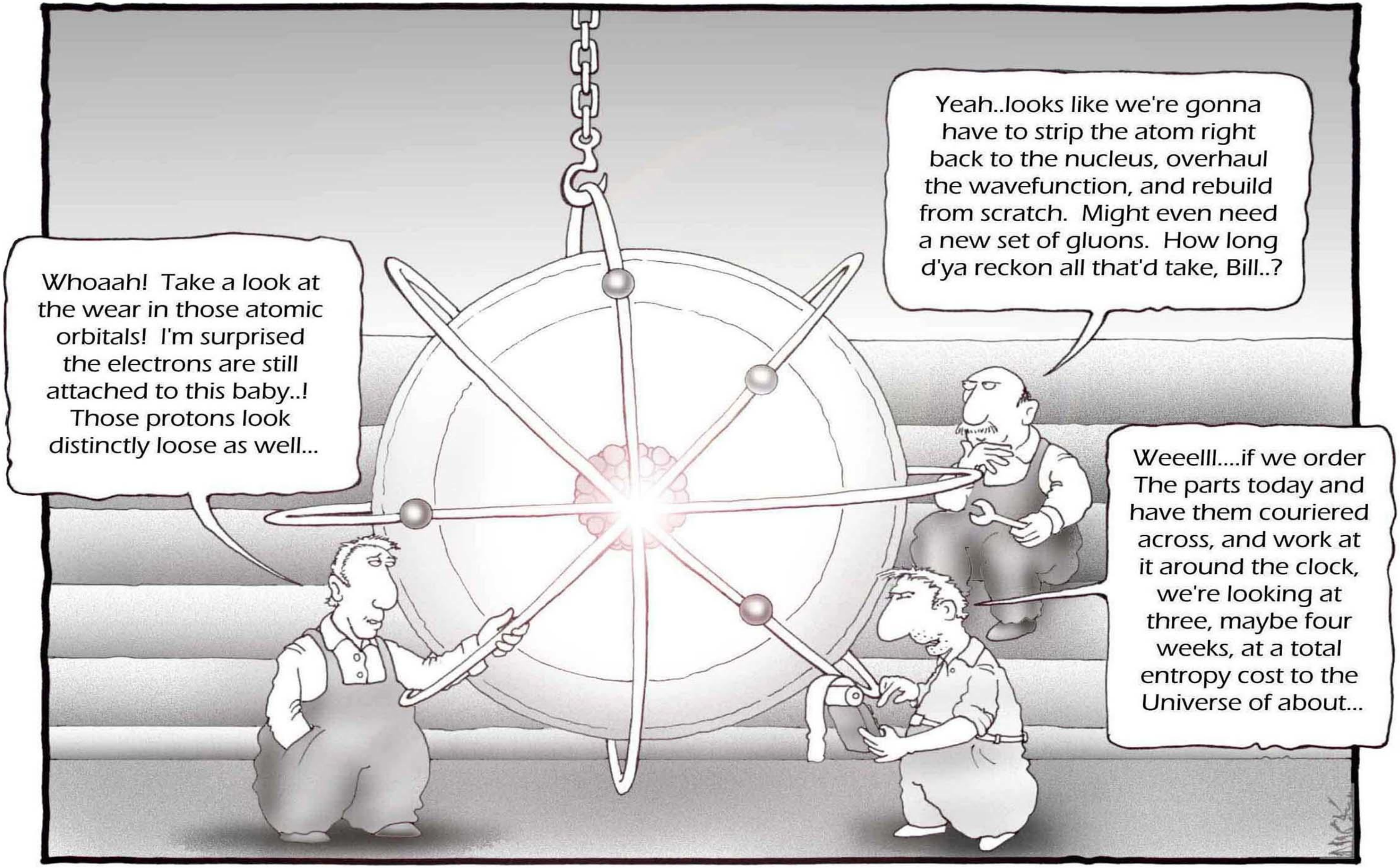


• A cloud of *delocalised π-bonding electrons* exists above and below the plane of the benzene ring.

The Modern Structure of Benzene



- Benzene is a regular, planar hexagon in which all of the bond angles are *120°* and all of the carbon-to-carbon covalent bond lengths are *0.139 nm*.



Quantum mechanics.

Quantum Theory of Atomic Structure

Presentation on
Quantum Theory of Atomic Structure
by Dr. Chris Slatter
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15th September 2005 – Raffles Girls' School (Secondary)
Updated 3rd October 2015 – Nanyang Girls' High School
Updated 21st September 2025 – Nanyang Girls' High School