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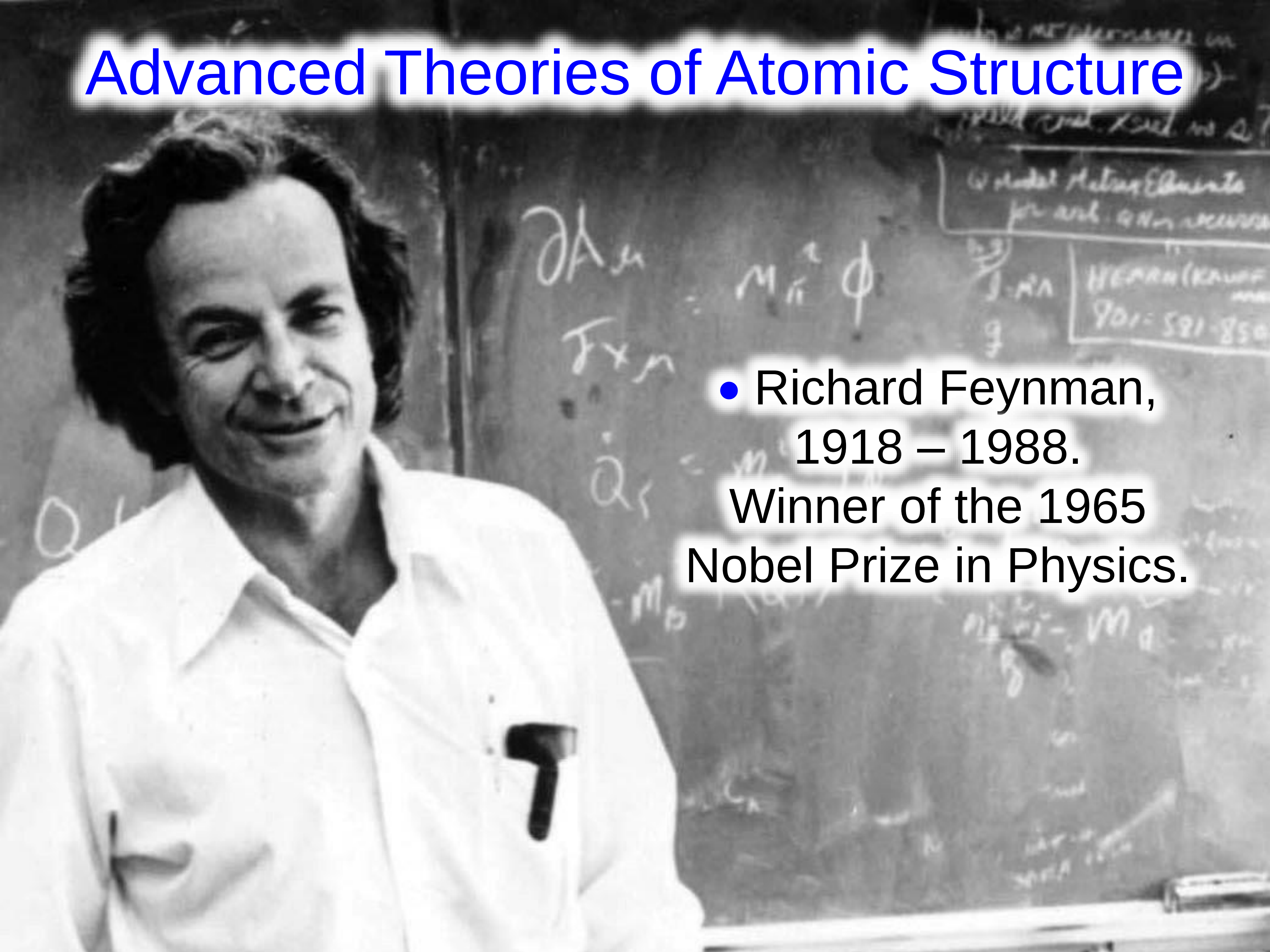
Nanyang 1917-2017

Advanced Theories of Atomic Structure: Atomic Orbitals

What are the more advanced theories of atomic structure?

Advanced Theories of Atomic Structure



- Richard Feynman, 1918 – 1988. Winner of the 1965 Nobel Prize in Physics.

Advanced Theories of Atomic Structure

- The modern scientific understanding of atomic structure – in which electrons are assumed to behave like *waves*, and orbit the nucleus of the atom in *atomic orbitals* – is based on *quantum mechanics*.

- Quantum mechanics is the branch of physics that deals with mathematical descriptions of how subatomic particles behave and interact.

- Richard Feynman introduced volume III of *The Feynman Lectures on Physics* with the words: “*I think I can safely say that nobody understands quantum mechanics*”.

Advanced Theories of Atomic Structure

- At the beginning of his classic undergraduate textbook series *The Feynman Lectures on Physics*, Richard Feynman felt the need to be perfectly honest about the counterintuitive nature of quantum theory. Subatomic particles, Feynman wrote, "*do not behave like waves, they do not behave like particles, they do not behave like clouds or billiard balls, or weights, or springs, or like anything that you have ever seen*."

Advanced Theories of Atomic Structure

- Fortunately, following the rules of quantum mechanics is far simpler than trying to visualise what they actually mean. The ability to follow through the consequences of a particular set of assumptions carefully, without getting too hung up on the philosophical implications, is one of the most important skills a scientist can learn.

- When deriving theories related to quantum mechanics, scientists set out their initial assumptions and compute their consequences. If they arrive at a set of predictions that agree with their observations of the natural world around them, then they accept the theory as good.

Advanced Theories of Atomic Structure

- Many problems in quantum mechanics are far too difficult to solve in a single mental leap, and deep understanding rarely emerges in *eureka* moments.

- The trick is for scientists to make sure that they understand each little step and, after a sufficient number of steps, the bigger picture starts to emerge. If this is not the case, then the scientists need to go back to the drawing board and start to derive a new theory.

- This is true for a scientific understanding of the atomic orbital structure of the atom. It should be attempted one step at-a-time until the big picture of how electrons orbit the nucleus of the atom starts to emerge.

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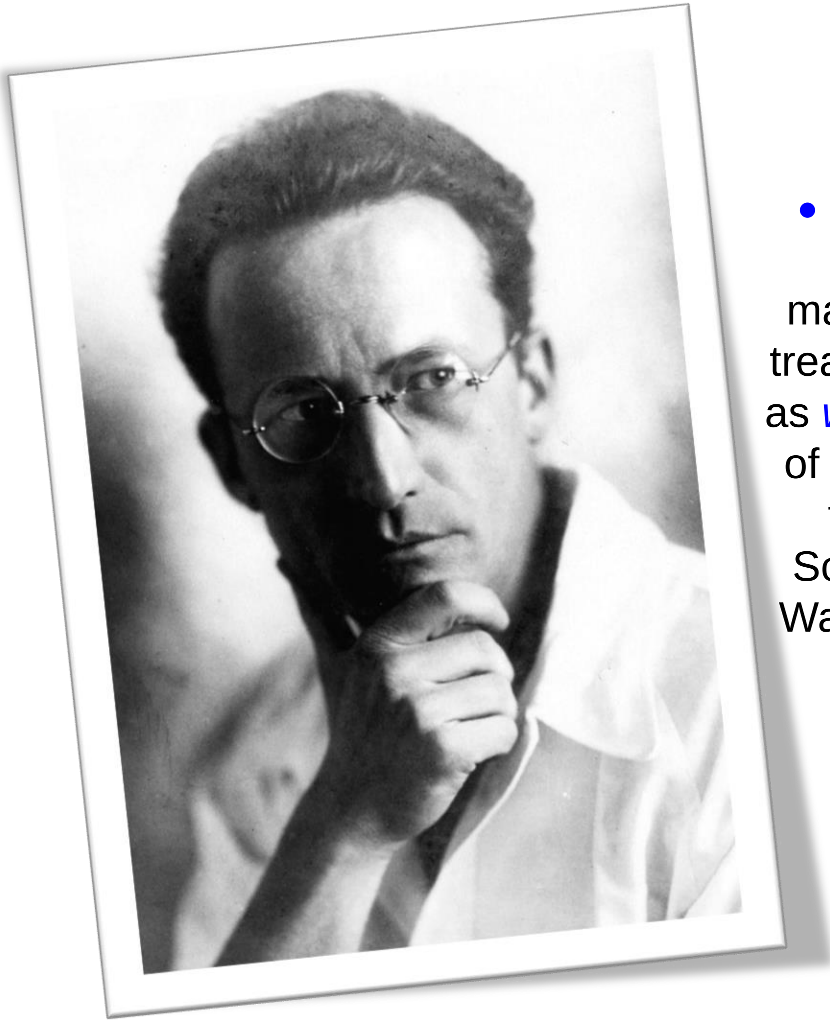
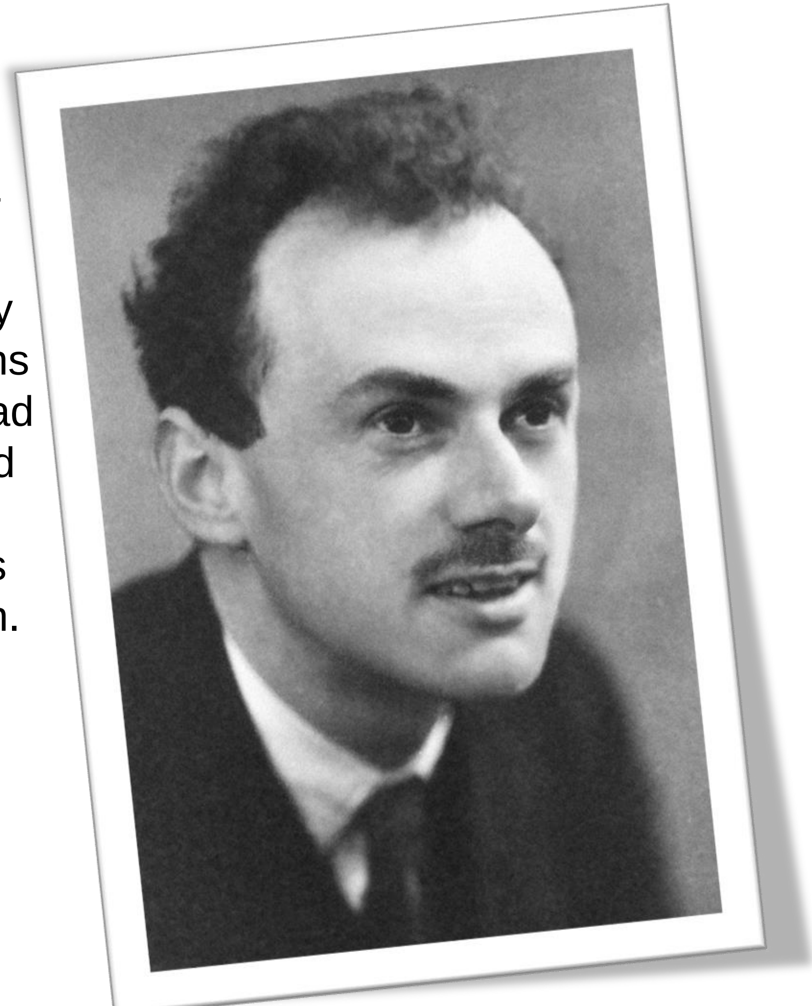


Erwin Schrödinger
1887 – 1961
Awarded the Nobel Prize for Physics in 1933.

- Schrödinger and Dirac mathematically treated electrons as *waves* instead of *particles* and formulated Schrödinger's Wave Equation.



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

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Schrödinger's Wave Equation

- In 1924, Louis de Broglie made the bold suggestion that *electrons* may have the properties of *waves* as well as the properties of *particles*.

- Schrödinger and Dirac mathematically treated *electrons* as *waves* instead of *particles* and formulated Schrödinger's Wave Equation.

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

- Graphical solutions for this complex equation give rise to *atomic orbitals.*

Advanced Theories of Atomic Structure

Atomic Orbitals

- An atomic orbital is the volume of space around the nucleus of an atom in which there is a high probability (*95%*) of finding an electron.

- An atomic orbital can hold a maximum number of *two* electrons.

- The location of an electron in an atom (*i.e.* which atomic orbital it belongs to) is given by *four electronic quantum numbers*.

- *Pauli's Exclusion Principle* states that no two electrons in the same atom can have the same set of electronic quantum numbers.

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- In simple terms, the four electronic quantum numbers are:

$\rightarrow$ First (n): Principle quantum number – the principle quantum shell that the electron occupies.

$\rightarrow$ Second (l): The sub-shell within the quantum shell that the electron occupies, *e.g. s-orbitals*, *p-orbitals* or *d-orbitals*.

$\rightarrow$ Third (m): The orbital within the sub-shell that the electron occupies, *e.g. p-orbitals* are always arranged in groups of three, so if an electron occupies a *p-orbital*, this electronic quantum number states exactly which one, the p_x*-orbital*, the p_y*-orbital* or the p_z*-orbital*.

$\rightarrow$ Fourth (s): For two electrons to occupy exactly the same orbital, they must have *opposite spin*. This electronic quantum number (spin quantum number) states whether the electron has a spin of $+^1/_2$ or $-^1/_2$.

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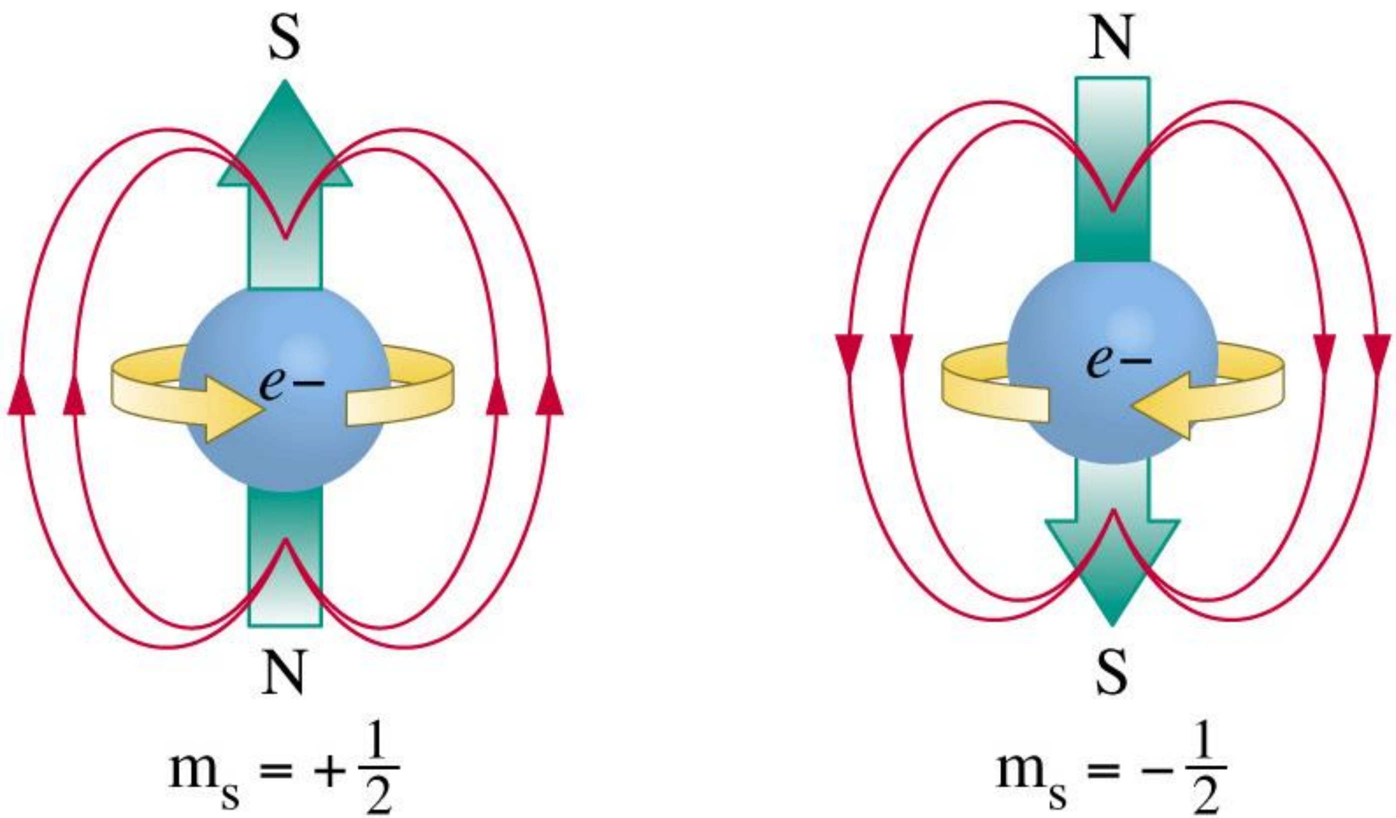

→ Fourth (*s*): For two electrons to occupy exactly the same orbital, they must have *opposite spin*. This electronic quantum number (spin quantum number) states whether the electron has a spin of $+^1/_2$ or $-^1/_2$.

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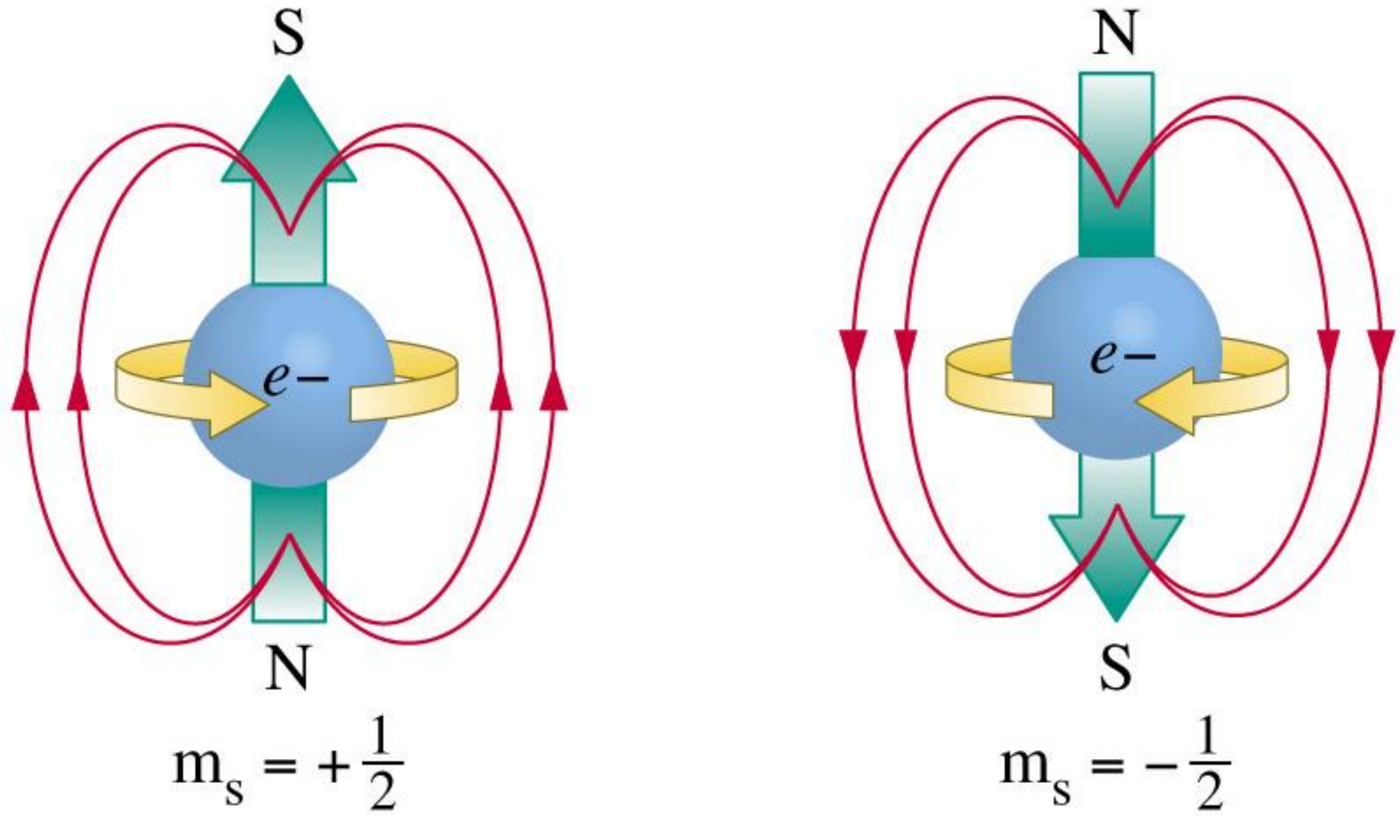

→ Fourth (s): The *spin quantum number* describes the *intrinsic angular momentum* of the electron. Because angular momentum is a *vector quantity*, it has both *magnitude* ($^1/_2$) and *direction* (either + or –).

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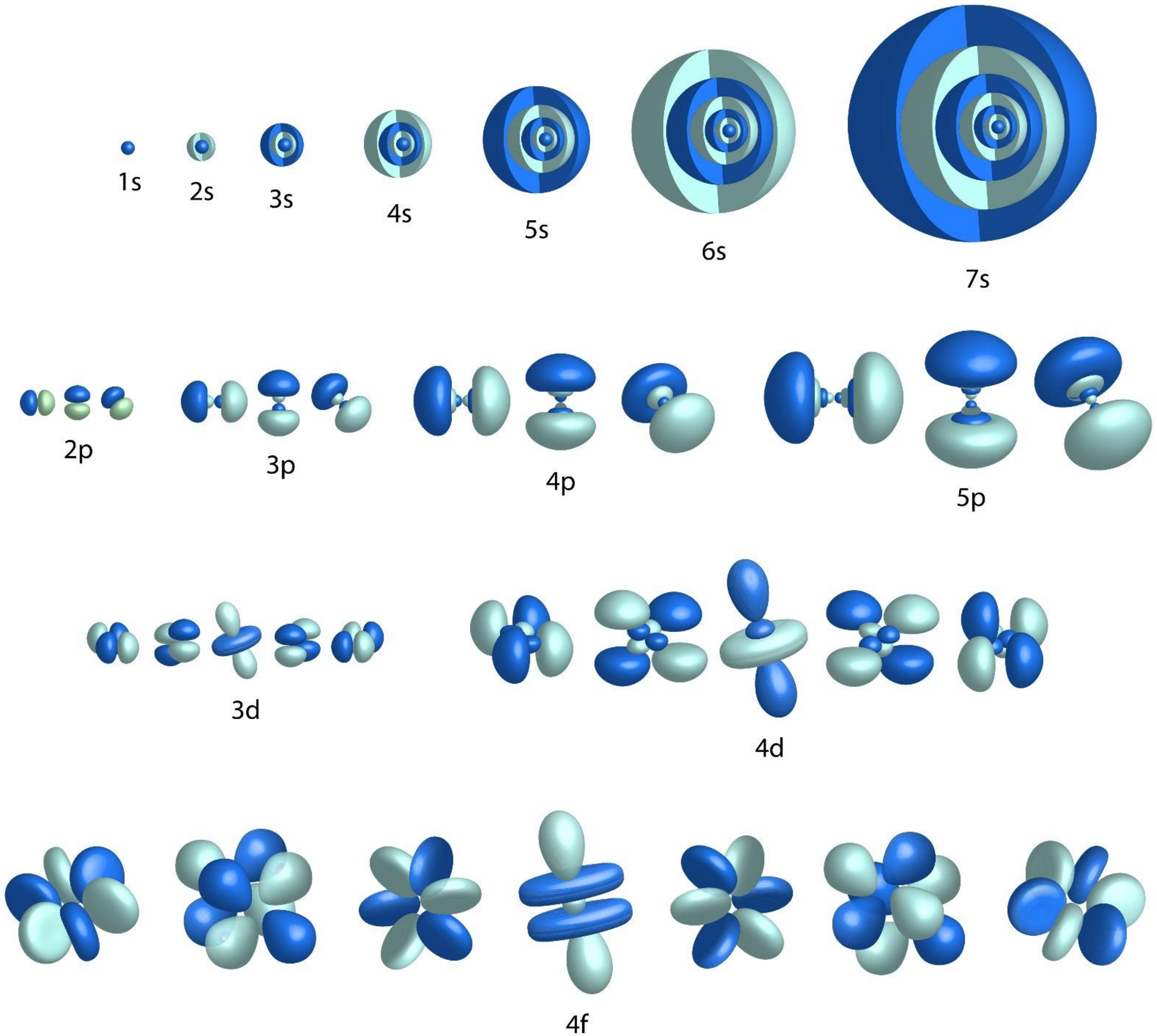

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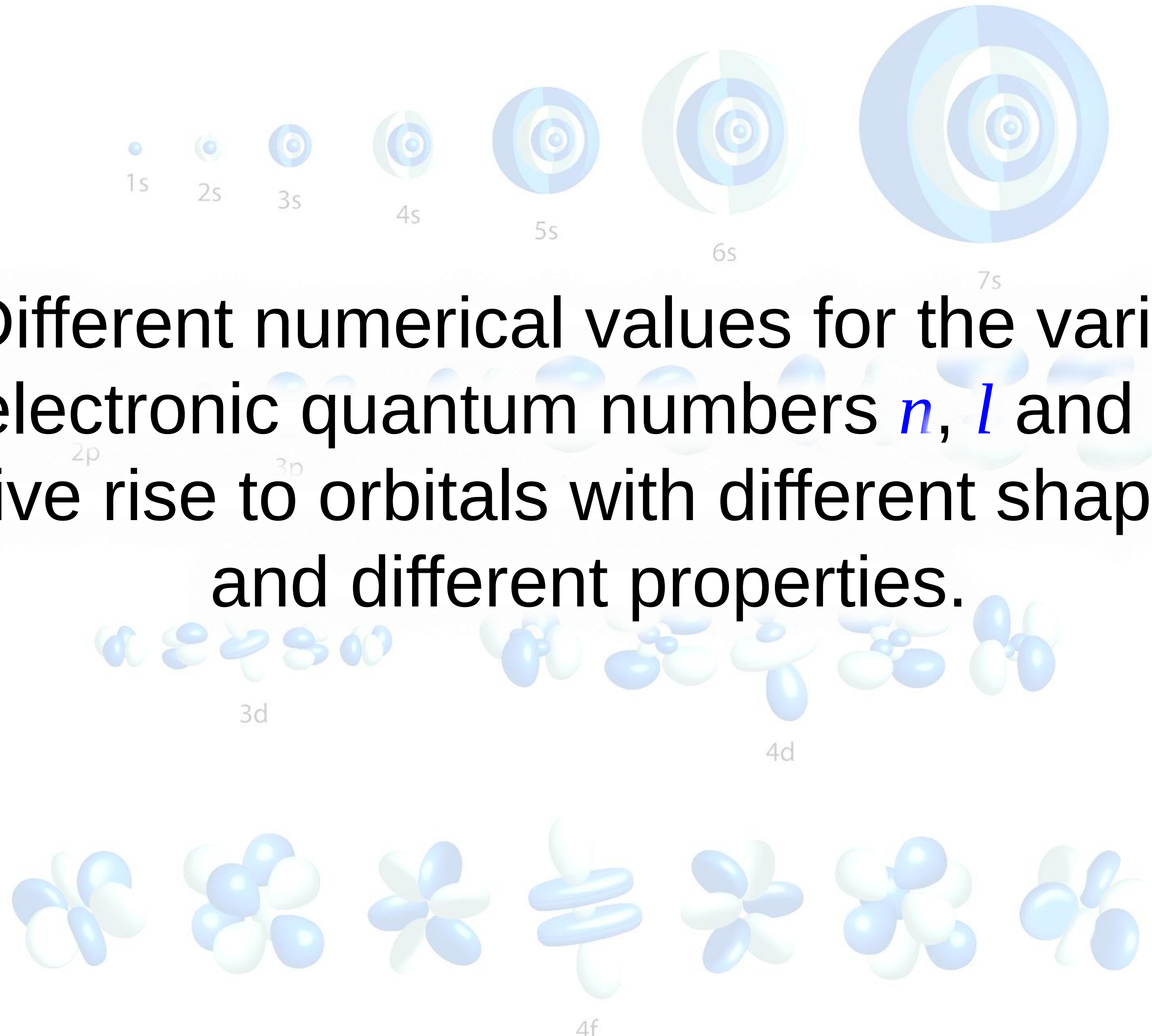

- Different numerical values for the various electronic quantum numbers n, l and m give rise to orbitals with different shapes and different properties.

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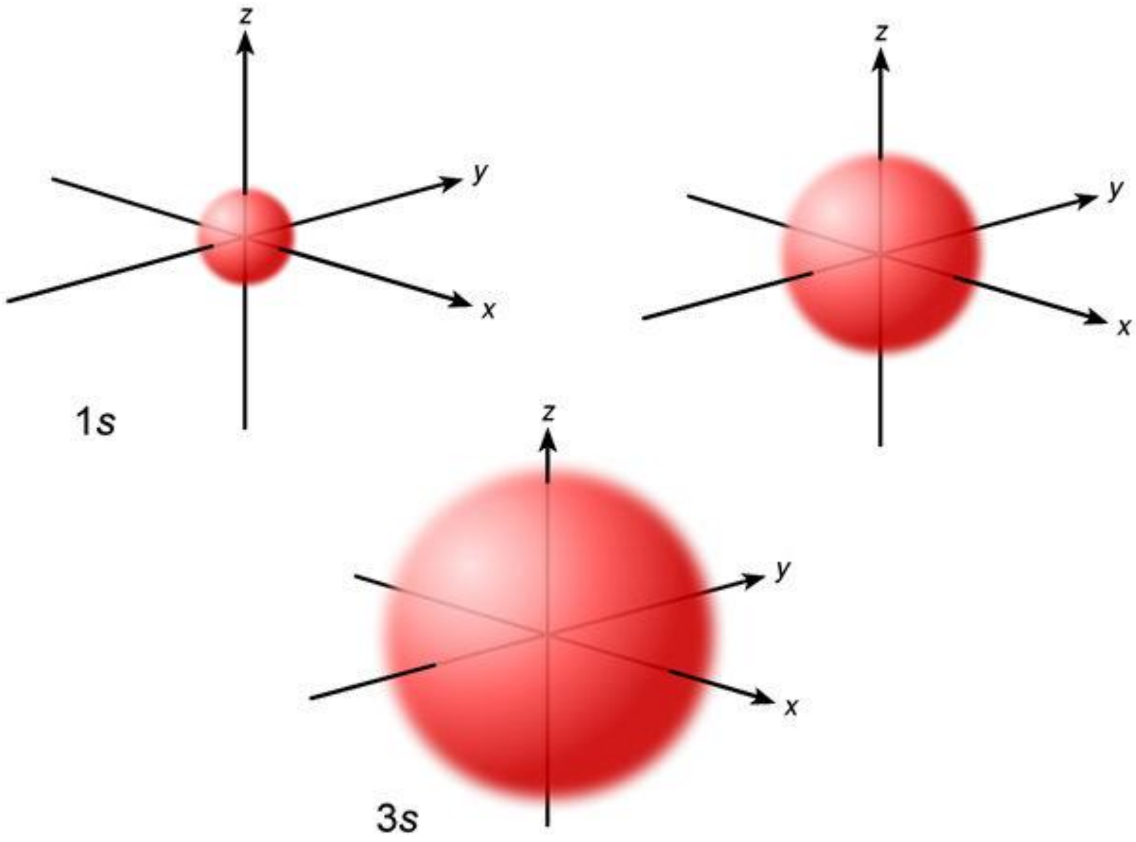

- A graphical solution to Schrödinger's Wave Equation – *s-orbitals*.

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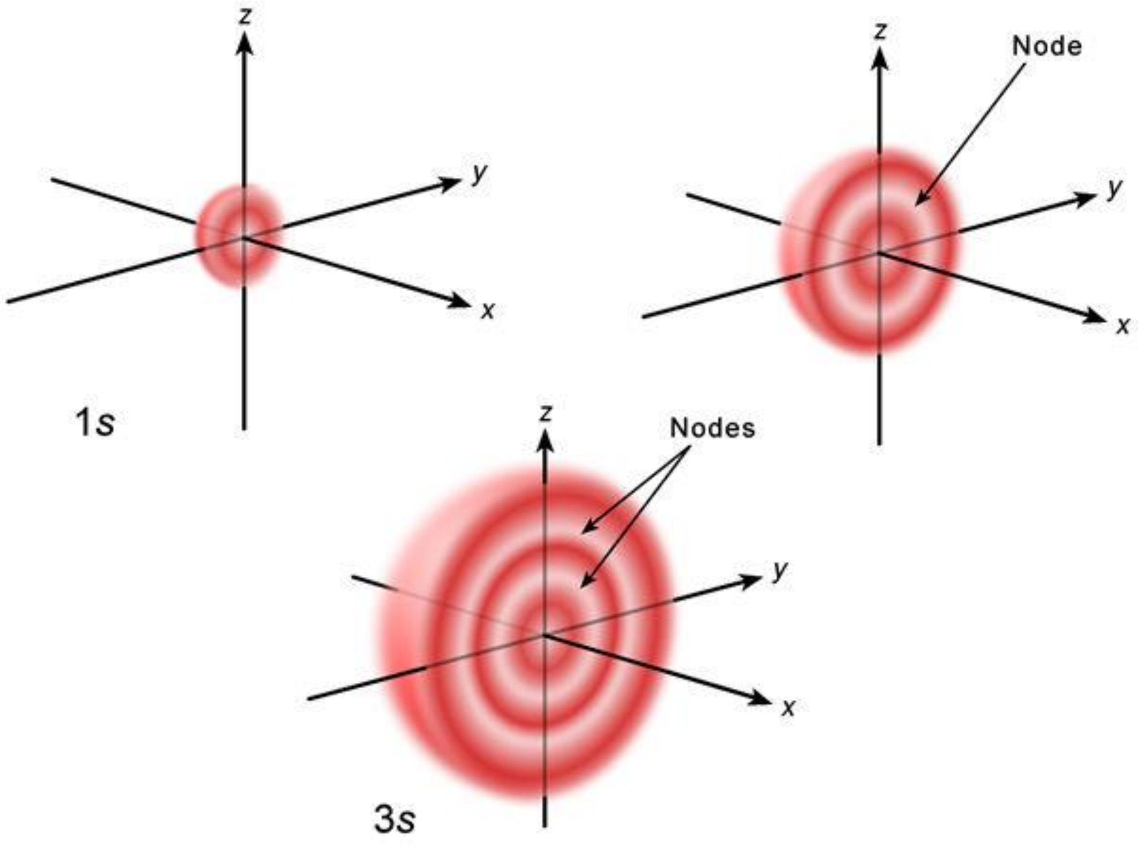

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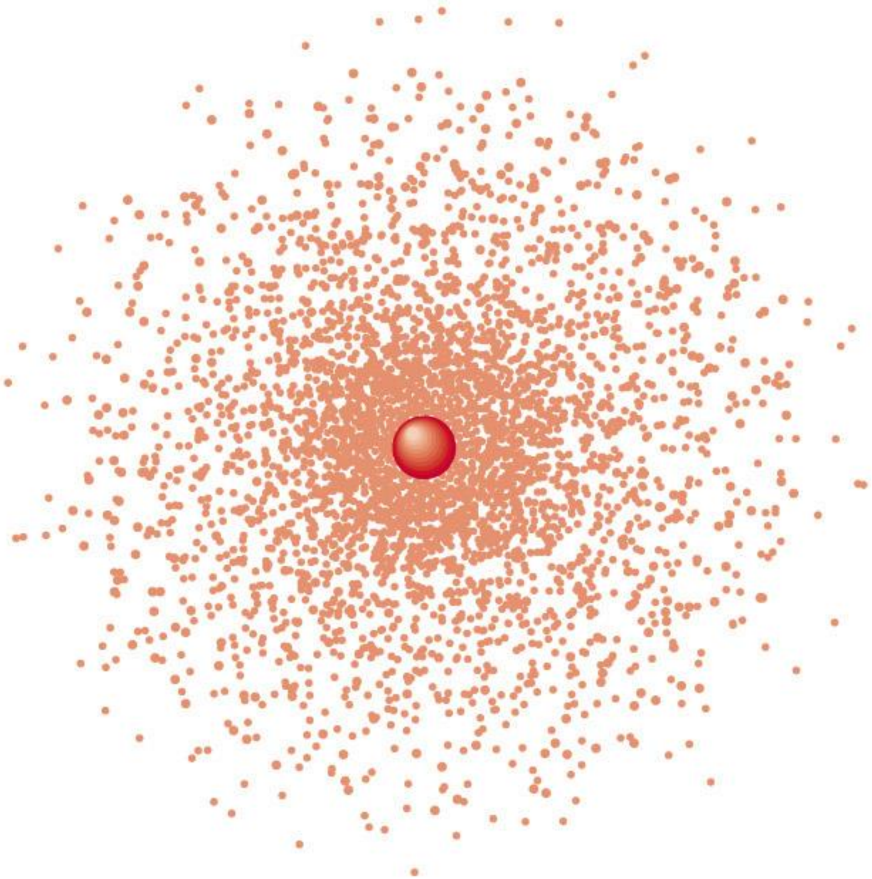

- An *s-orbital*. The closer the dots are placed together, the greater the probability of an electron being located at that position.

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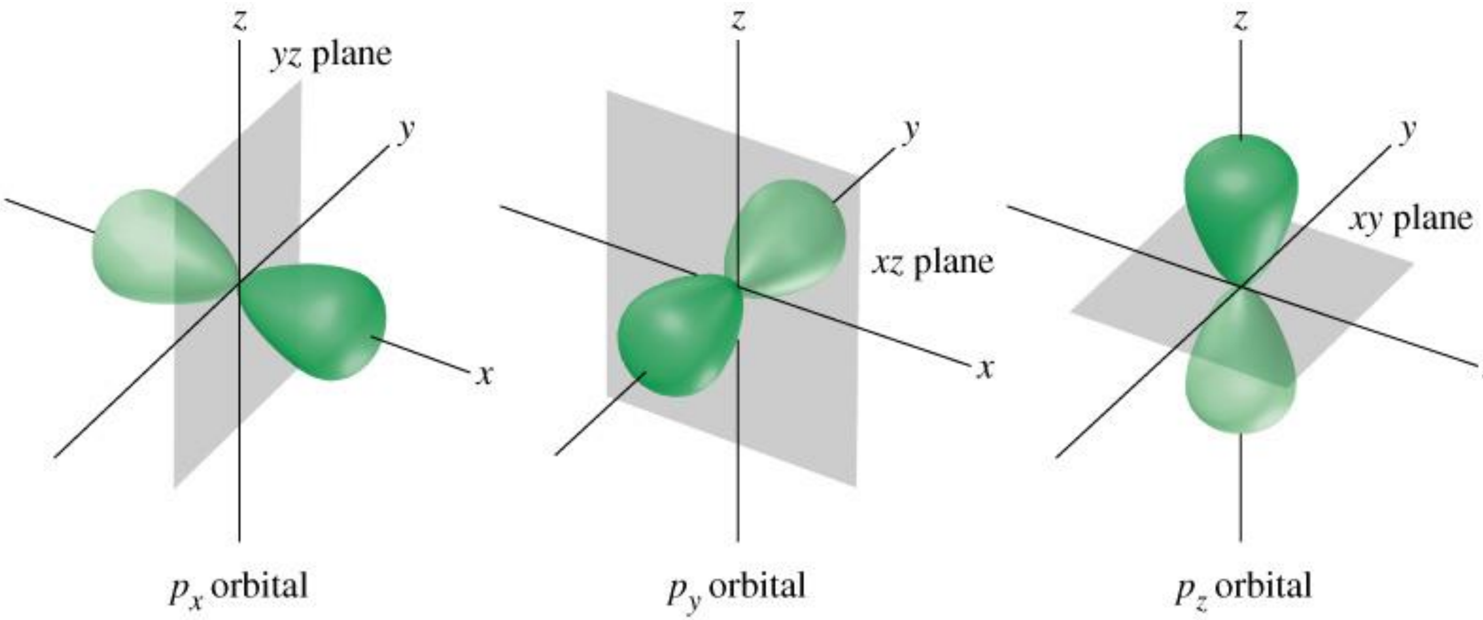

- A graphical solution to Schrödinger's Wave Equation – *p-orbitals*. The orbitals have been drawn separately for clarity. In reality, it is assumed that the three *p*-orbitals are superimposed on top of each other.

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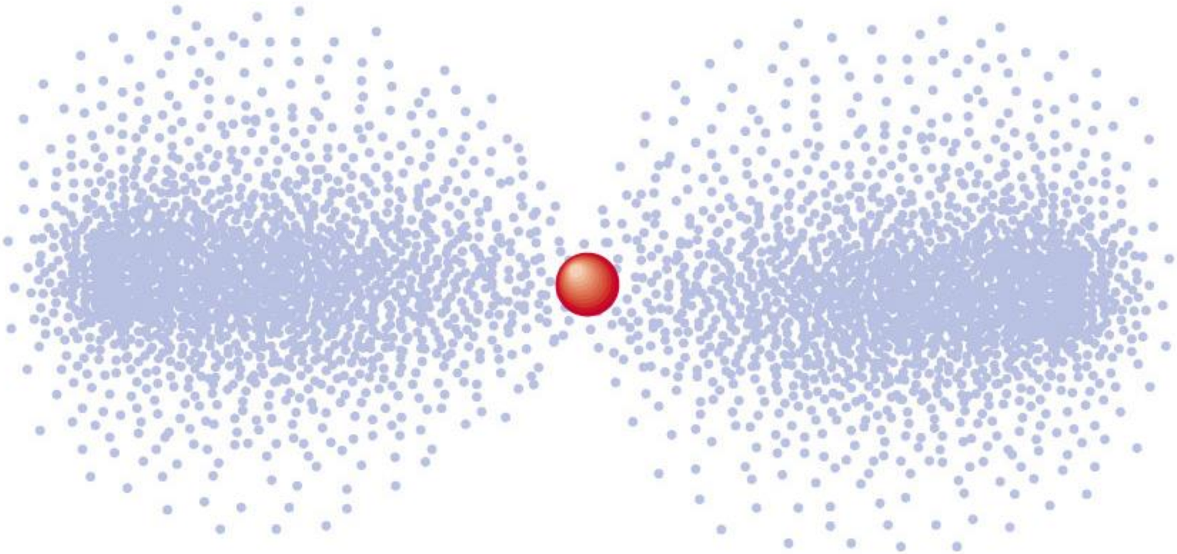

- A *p-orbital*. The closer the dots are placed together, the greater the probability of an electron being located at that position.

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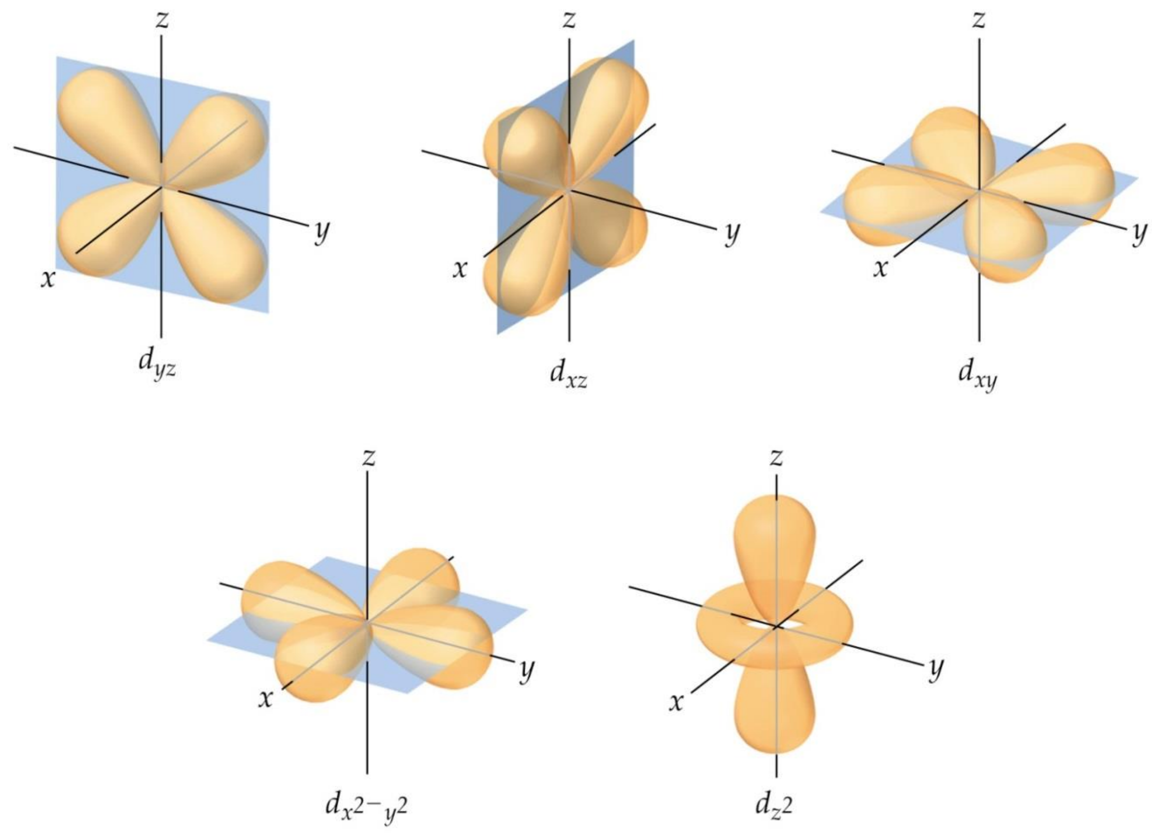

- A graphical solution to Schrödinger's Wave Equation – *d-orbitals*. The orbitals have been drawn separately for clarity. In reality, it is assumed that the five *d*-orbitals are superimposed on top of each other.

Advanced Theories of Atomic Structure

Enrichment: A Brief Note About the Values of the Four Electronic Quantum Numbers

• The electronic quantum number n takes on integer values (n = 1, 2, 3, and so on) and the energy of the electron increases as the value of n increases.

• The electronic quantum number l must be an integer that is smaller than n. The electronic quantum number l can equal 0, but cannot have a value that is negative. For example, if $n = 4$, then l can be equal to 0, 1, 2 or 3.

If $l = 0$, an *s*-orbital is present.

If $l = 1$, a group of *p*-orbitals are present.

If $l = 2$, a group of *d*-orbitals are present.

If $l = 3$, a group of *f*-orbitals are present.

Advanced Theories of Atomic Structure

Enrichment: A Brief Note About the Values of the Four Electronic Quantum Numbers

- The electronic quantum number m can equal any value from negative l to positive l in integer steps. For example, if l = 2, then m can be equal to –2, –1, 0, +1 or +2.

- If n = 1, then how many different atomic orbitals are there? Applying the rules, if n = 1, then l must equal 0 and m must also equal 0. So, when n has a value of 1, there is only one atomic orbital (one *s*-orbital).

Advanced Theories of Atomic Structure

Enrichment: A Brief Note About the Values of the Four Electronic Quantum Numbers

• If n = 2, then how many different atomic orbitals are there? Applying the rules, if n = 2, then l can have values of 0 or 1.

$\rightarrow$ If l = 0, then m must also equal 0 (one *s*-orbital).

$\rightarrow$ If l = 1, then m can have values of –1, 0 or +1 (three *p*-orbitals).

So, when n has a value of 2, there are a total of four atomic orbitals (one *s*-orbital and three *p*-orbitals).

Advanced Theories of Atomic Structure

Enrichment: A Brief Note About the Values of the Four Electronic Quantum Numbers

• If n = 3, then how many different atomic orbitals are there? Applying the rules, if n = 3, then l can have values of 0, 1 or 2.

→ If l = 0, then m must also equal 0 (one *s*-orbital).

→ If l = 1, then m can have values of –1, 0 or +1 (three *p*-orbitals).

→ If l = 2, them m can have values of –2, –1, 0, +1 or +2 (five *d*-orbitals).

So, when n has a value of 3, there are a total of nine atomic orbitals (one *s*-orbital, three *p*-orbitals and five *d*-orbitals).

Advanced Theories of Atomic Structure

Enrichment: A Brief Note About the Values of the Four Electronic Quantum Numbers

• If n = 4, then how many different atomic orbitals are there?

Applying the rules, if n = 4, then l can have values of 0, 1, 2 or 3.

→ If l = 0, then m must also equal 0 (one *s*-orbital).

→ If l = 1, then m can have values of –1, 0 or +1 (three *p*-orbitals).

→ If l = 2, them m can have values of –2, –1, 0, +1 or +2 (five *d*-orbitals).

→ If l = 3, then m can have values of –3, –2, –1, 0, +1, +2 or +3 (seven *f*-orbitals).

So, when n has a value of 4, there are a total of sixteen atomic orbitals (one *s*-orbital, three *p*-orbitals, five *d*-orbitals and seven *f*-orbitals).

Advanced Theories of Atomic Structure

Enrichment: A Brief Note About the Values of the Four Electronic Quantum Numbers

- The total number of electrons that can occupy an electron shell is given by the formula:

$$\text{Electrons} = 2n^2$$

$\rightarrow$ For $n = 1$, electrons = $2 \times 1^2 = 2 \times 1 = 2\ e^-$

This is the 1s orbital ($2\ e^-$)

$\rightarrow$ For $n = 2$, electrons = $2 \times 2^2 = 2 \times 4 = 8\ e^-$

These are the 2s ($2\ e^-$) + 2p ($6\ e^-$) orbitals

$\rightarrow$ For $n = 3$, electrons = $2 \times 3^2 = 2 \times 9 = 18\ e^-$

These are the 3s ($2\ e^-$) + 3p ($6\ e^-$) + 3d ($10\ e^-$) orbitals

$\rightarrow$ For $n = 4$, electrons = $2 \times 4^2 = 2 \times 16 = 32\ e^-$

These are the 4s ($2\ e^-$) + 4p ($6\ e^-$) + 4d ($10\ e^-$) + 4f ($14\ e^-$) orbitals

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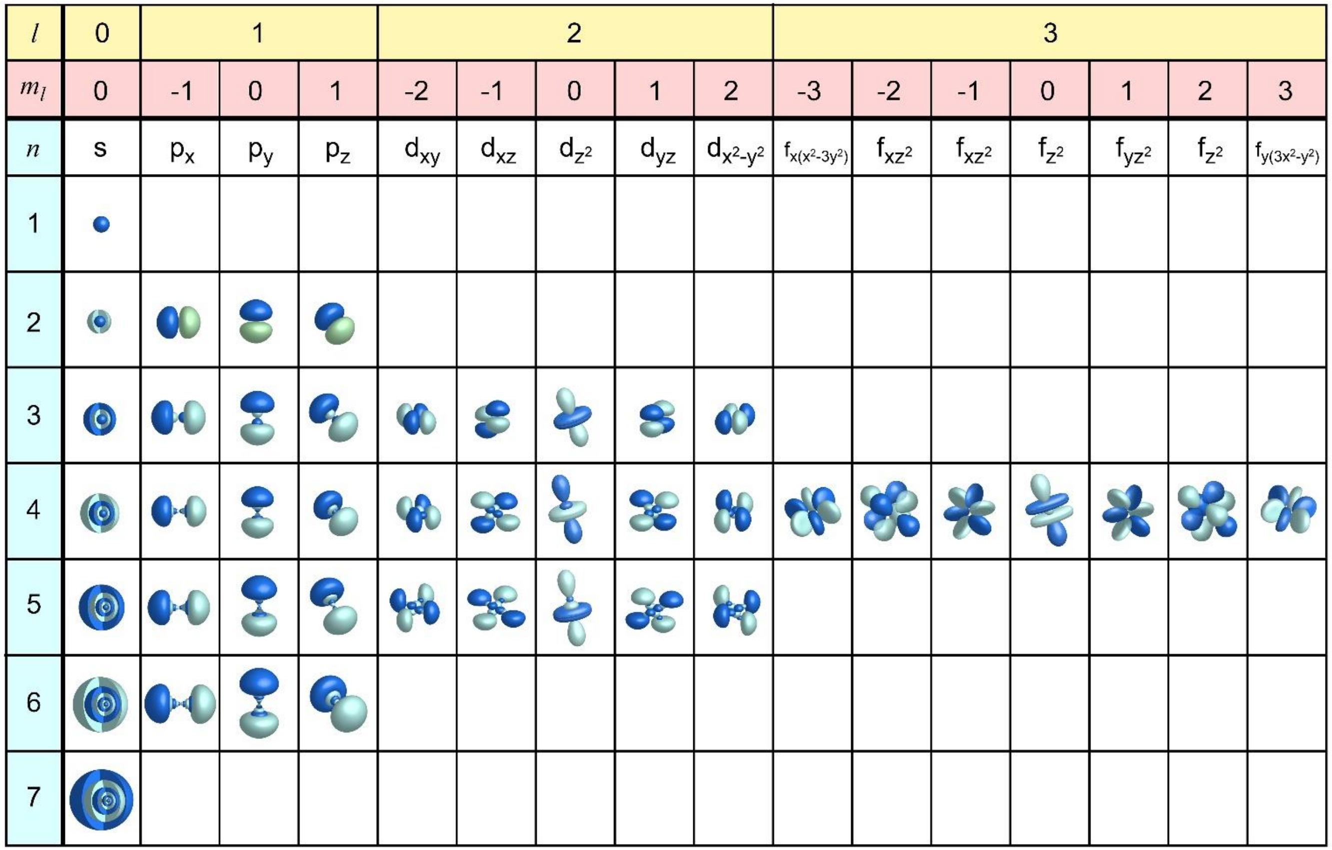
Shapes and Occurrence of Atomic Orbitals



- Diagram showing the various orbitals that arise from different values of the electronic quantum numbers n, l and m.

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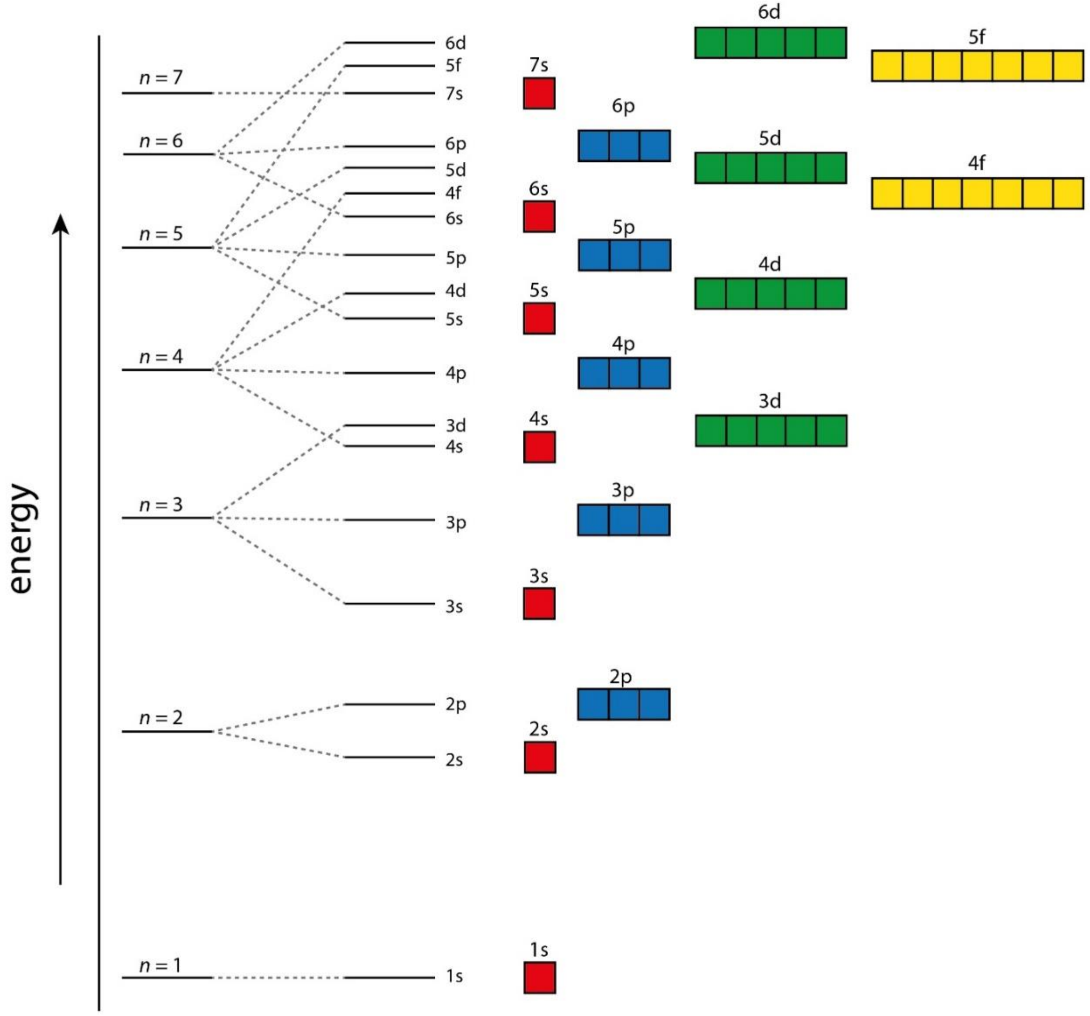

- Diagram showing the energy levels of the various orbitals.

Note: Orbitals fill from the lowest energy to the highest energy.

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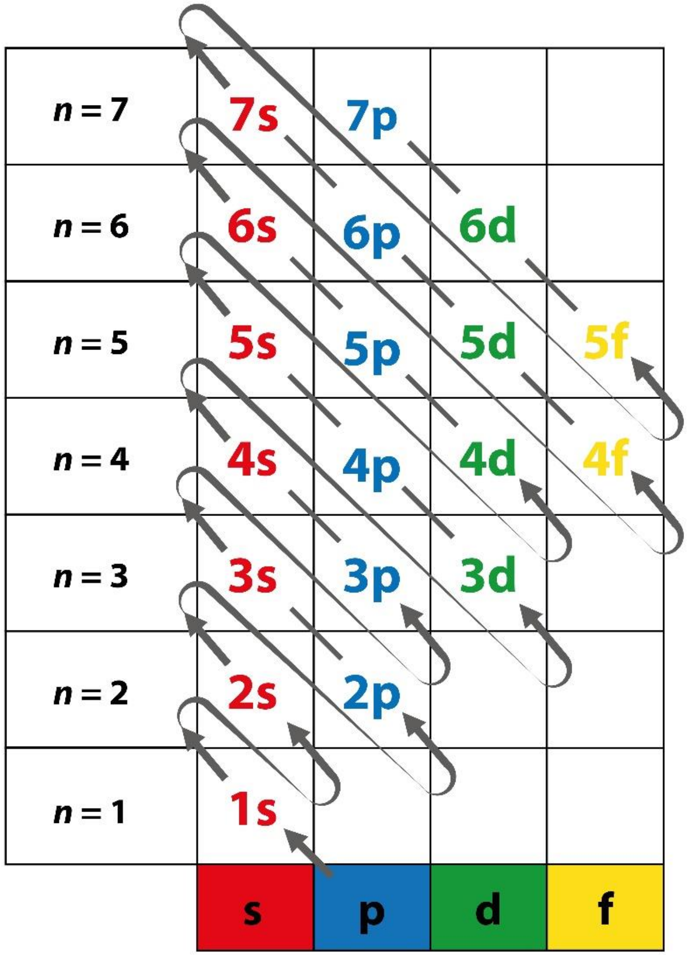

- Diagram showing the order in which atomic orbitals fill-up with electrons.

Advanced Theories of Atomic Structure

Rules for Filling Atomic Orbitals

• Heisenberg's Uncertainty Principle – It is not possible to determine both the position and the momentum of an electron at the same time. This gives rise to the idea that an electron's position in an atom is *uncertain*, and therefore scientists can only identify where there is the *highest probability* of finding an electron – which is how the atomic orbital is defined.

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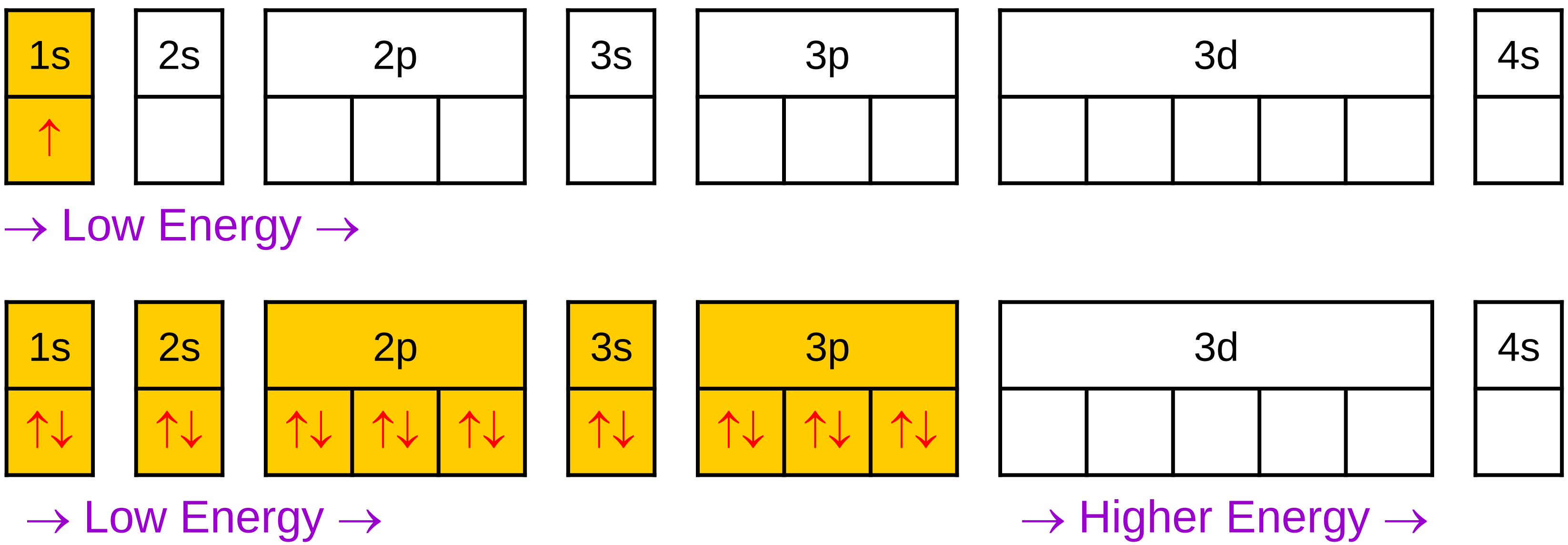
Rules for Filling Atomic Orbitals

- The Aufbau Principle – Electrons fill-up atomic orbitals from the lowest energy to the highest energy. Left undisturbed, objects will tend to their lowest possible energy.



Advanced Theories of Atomic Structure

Rules for Filling Atomic Orbitals

• Pauli's Exclusion Principle – No two electrons within the same atom can have the same values for all four quantum numbers, *i.e.* every electron in the same atom must have a unique combination of quantum numbers. As a consequence, electrons in the same orbital must spin in opposite directions. In atomic orbital diagrams, the spin quantum number is represented by an arrow (↑ or ↓). Two arrows pointing in opposite directions represent two electrons with opposite spin (↑ and ↓).

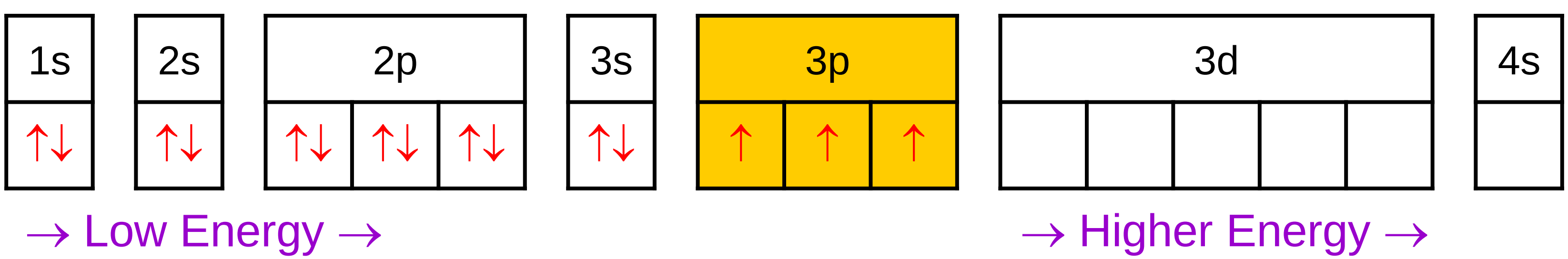
1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

→ Low Energy → → Higher Energy →

Advanced Theories of Atomic Structure

Rules for Filling Atomic Orbitals

• Hund's Rule of Maximum Multiplicity – When placed in atomic orbitals of equal energy, electrons will remain unpaired. Electrons carry a charge of –1. There will be an electrostatic force of repulsion between electrons in the same orbital. Placing electrons in different atomic orbitals of the same energy will reduce the electrostatic force of repulsion between the electrons and make the system more stable.



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Shapes and Occurrence of Atomic Orbitals

- Each principle quantum shell is divided into one or more sub-shells.

Principle Quantum Shell (n)	Sub-shell (l)	Maximum Number of Electrons
1	1*s*	2
2	2*s*, 2*p*	8
3	3*s*, 3*p*, 3*d*	18
4	4*s*, 4*p*, 4*d*, 4*f*	32

Advanced Theories of Atomic Structure

Shapes and Occurrence of Atomic Orbitals

- There are four sub-shells, arranged in increasing energy s $\rightarrow$ p $\rightarrow$ d $\rightarrow$ f. Each sub-shell holds a different number of electrons

Principle Quantum Shell (*n*)	Sub-shell (*l*)	Maximum Number of Electrons
1	1*s*	2
2	2*s*, 2*p*	8
3	3*s*, 3*p*, 3*d*	18
4	4*s*, 4*p*, 4*d*, 4*f*	32

Advanced Theories of Atomic Structure

Shapes and Occurrence of Atomic Orbitals

Orbital	Shape	Occurrence
s (*sharp*)	spherical	**1** in every principle level
p (*principle*)	dumb-bell or hour glass	**3** in every level from **2** onwards
d (*diffuse*)	complex and various	**5** in every level from **3** onwards
f (*fundamental*)	complex and various	**7** in every level from **4** onwards

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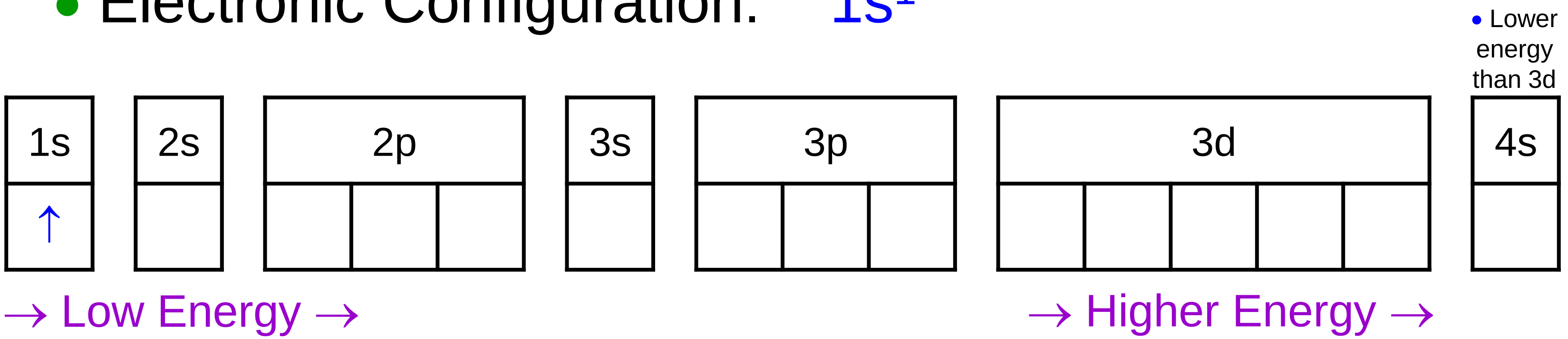
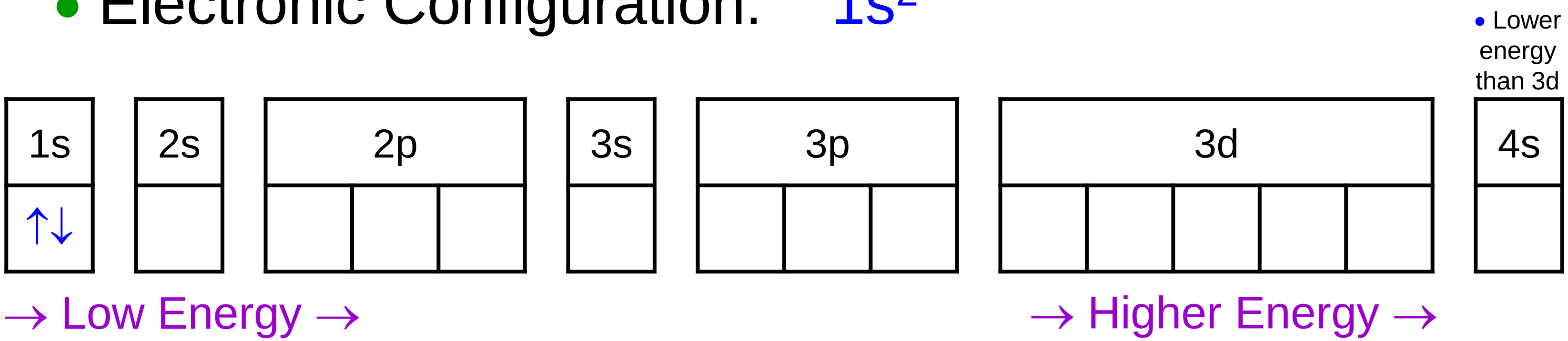
- Atomic Number: 1
- Name: Hydrogen
- Symbol: H
- Electronic Configuration: $1s^1$



- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.

Advanced Theories of Atomic Structure

- Atomic Number: 2
- Name: Helium
- Symbol: He
- Electronic Configuration: $1s^2$



- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.

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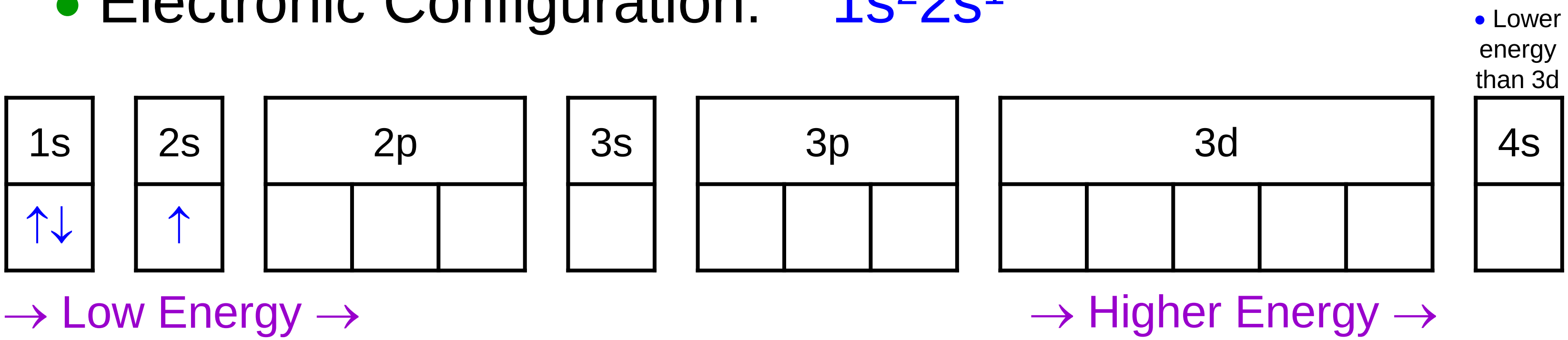
- Atomic Number: 3
- Name: Lithium
- Symbol: Li
- Electronic Configuration: $1s^2 2s^1$

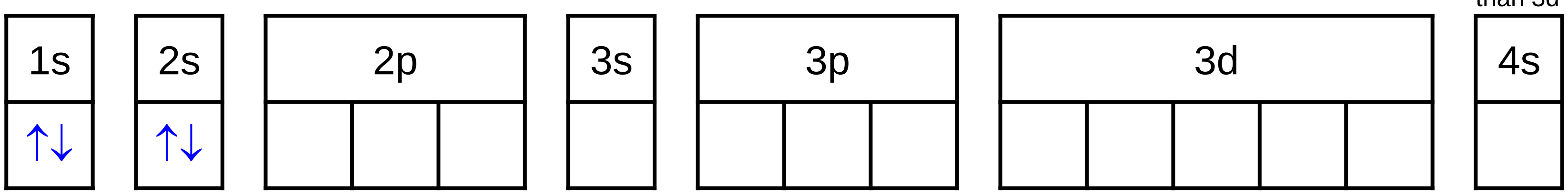


- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.

Advanced Theories of Atomic Structure

- Atomic Number: 4
- Name: Beryllium
- Symbol: Be
- Electronic Configuration: $1s^2 2s^2$

- Lower energy than 3d



→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
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Advanced Theories of Atomic Structure

- Atomic Number: 5
- Name: Boron
- Symbol: B
- Electronic Configuration: $1s^2 2s^2 2p^1$

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑												

• Lower energy than 3d

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.

Advanced Theories of Atomic Structure

- Atomic Number: 6
- Name: Carbon
- Symbol: C
- Electronic Configuration: $1s^22s^22p^2$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑	↑											

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 7
- Name: Nitrogen
- Symbol: N
- Electronic Configuration: $1s^2 2s^2 2p^3$

- Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑	↑	↑										

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 8
- Name: Oxygen
- Symbol: O
- Electronic Configuration: $1s^22s^22p^4$

- Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑	↑										

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

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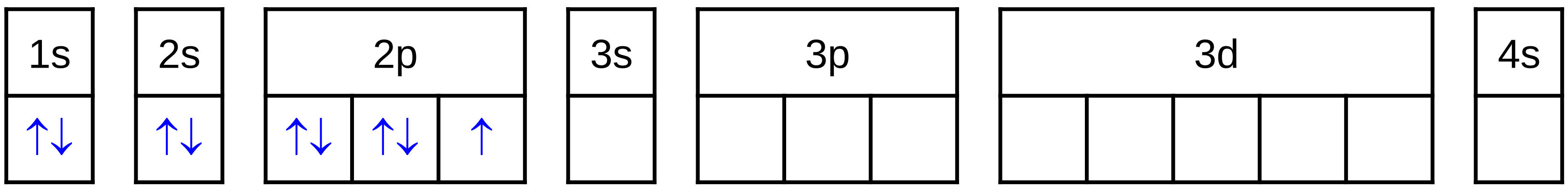
- Atomic Number: 9
- Name: Fluorine
- Symbol: F
- Electronic Configuration: $1s^2 2s^2 2p^5$

- Lower energy than 3d



→ Low Energy →

→ Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

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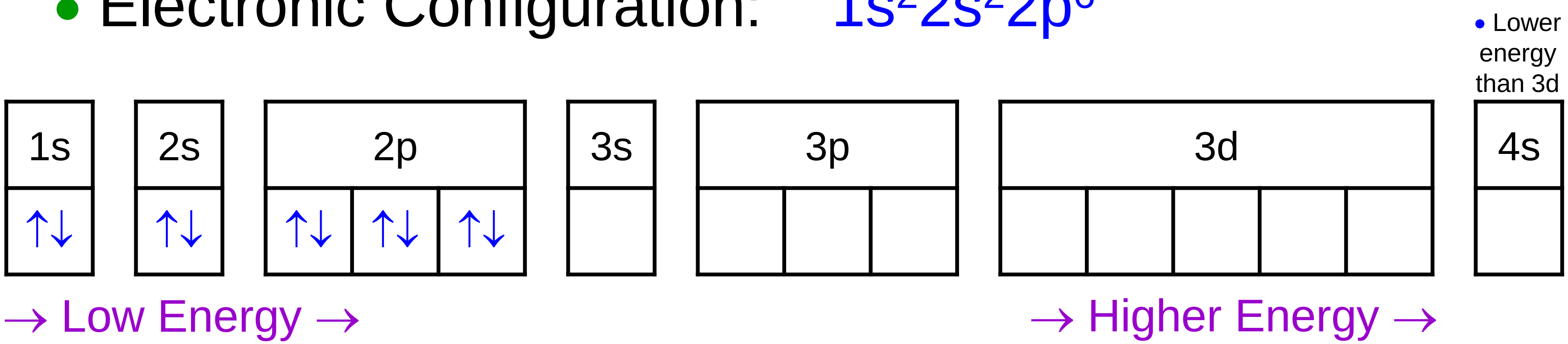
- Atomic Number: 10
- Name: Neon
- Symbol: Ne
- Electronic Configuration: $1s^2 2s^2 2p^6$



- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 11
- Name: Sodium
- Symbol: Na
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^1$

- Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑									

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 12
- Name: Magnesium
- Symbol: Mg
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓									

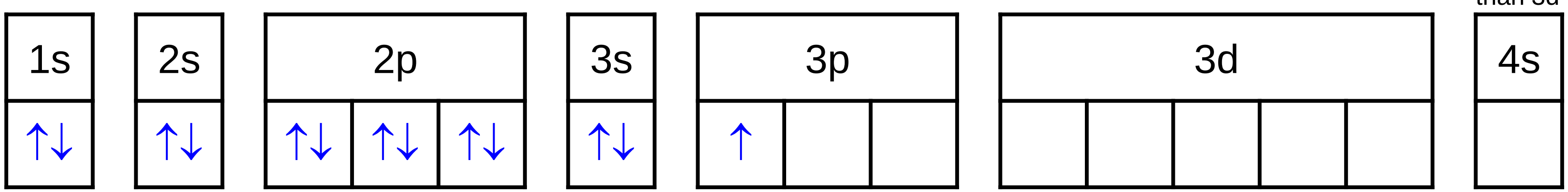
→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 13
- Name: Aluminium
- Symbol: A*l*
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^1$

- Lower energy than 3d



→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 14
- Name: Silicon
- Symbol: Si
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^2$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑							

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 15
- Name: Phosphorus
- Symbol: P
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^3$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑						

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 16
- Name: Sulfur
- Symbol: S
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^4$

- Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑						

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 17
- Name: Chlorine
- Symbol: C*l*
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^5$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑						

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 18
- Name: Argon
- Symbol: Ar
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓						

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 19
- Name: Potassium
- Symbol: K
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓						↑

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Why is the electronic configuration of *potassium*…

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓						↑

→ Low Energy → → Higher Energy →

…instead of…

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑					

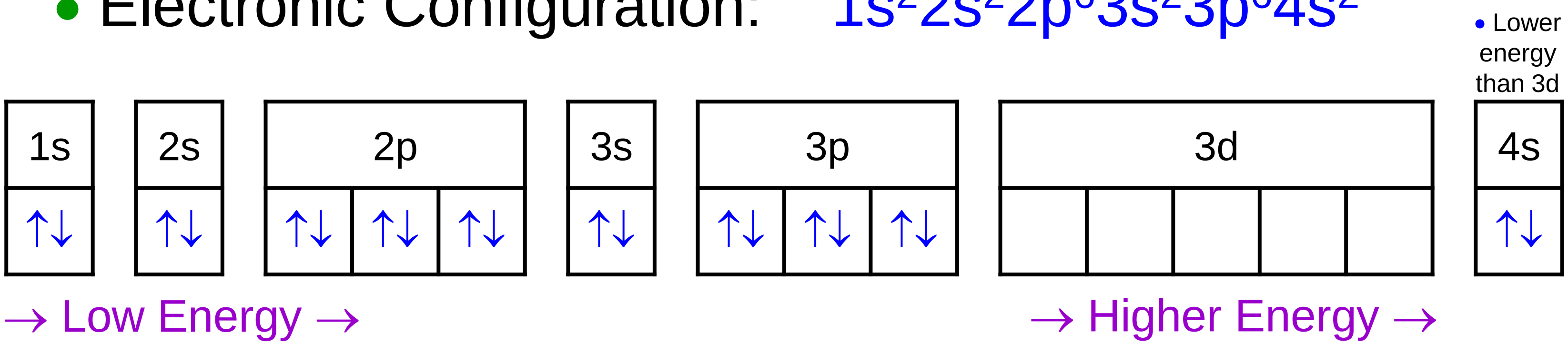
→ Low Energy → → Higher Energy →

- Although the 4s sub-shell is further from the nucleus than the 3d sub-shell, the 4s sub-shell is *lower in energy* than the 3d sub-shell.

- According to the Aufbau Principle (electrons fill-up atomic orbitals from lower energy to higher energy) the *lower energy* 4s sub-shell will fill with electrons before the *higher energy* 3d sub-shell.

Advanced Theories of Atomic Structure

- Atomic Number: 20
- Name: Calcium
- Symbol: Ca
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$



- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 21
- Name: Scandium
- Symbol: Sc
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$
  - Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑					↑↓

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 22
- Name: Titanium
- Symbol: Ti
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑				↑↓

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 23
- Name: Vanadium
- Symbol: V
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑			↑↓

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 24
- Name: Chromium
- Symbol: Cr
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑	↑

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Why is the electronic configuration of *chromium*…

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑	↑

→ Low Energy → → Higher Energy →

…instead of…

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑		↑↓

→ Low Energy → → Higher Energy →

- Completely filled sub-shells are *more stable* than partially filled sub-shells.
- A sub-shell that is exactly half-filled is *more stable* than a sub-shell that is not exactly half-filled.
- An electron in the 4s orbital is transferred to an empty 3d orbital so as to obtain two stable half-filled sub-shells ($3d^5$ and $4s^1$) instead of one incomplete sub-shell ($3d^4$) and one complete sub-shell ($4s^2$).

Advanced Theories of Atomic Structure

- Atomic Number: 25
- Name: Manganese
- Symbol: Mn
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑	↑↓

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 26
- Name: Iron
- Symbol: Fe
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$

- Lower energy than 3d

1s	2s	2p	3s	3p	3d	4s
↑↓	↑↓	↑↓ | ↑↓ | ↑↓	↑↓	↑↓ | ↑↓ | ↑↓	↑↓ | ↑ | ↑ | ↑ | ↑	↑↓

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 27
- Name: Cobalt
- Symbol: Co
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑↓

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 28
- Name: Nickel
- Symbol: Ni
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑↓

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Atomic Number: 29
- Name: Copper
- Symbol: Cu
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$.

• Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Why is the electronic configuration of *copper*…

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑

→ Low Energy → → Higher Energy →

…instead of…

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑↓

→ Low Energy → → Higher Energy →

- Completely filled sub-shells are *more stable* than partially filled sub-shells.
- A sub-shell that is exactly half-filled is *more stable* than a sub-shell that is not exactly half-filled.
- An electron in the 4s orbital is transferred to a 3d orbital so as to obtain one stable complete sub-shell ($3d^{10}$) and one stable half-filled sub-shell ($4s^{1}$) instead of one incomplete sub-shell ($3d^{9}$) and one complete sub-shell ($4s^{2}$).

Advanced Theories of Atomic Structure

- Atomic Number: 30
- Name: Zinc
- Symbol: Zn
- Electronic Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$. • Lower energy than 3d

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

→ Low Energy → → Higher Energy →

- Electrons are represented by *arrows* (↑ and ↓) which fill atomic orbitals that are represented by *boxes*.
- Electrons occupy atomic orbitals from the lowest energy to the highest energy. This is known as the *Aufbau Principle*.
- A single electron will occupy a single atomic orbital before two electrons are forced to *spin pair-up* with each other in the same orbital (*Hund's Rule*).

Advanced Theories of Atomic Structure

- Elements can be classified based upon their electronic configurations.

Group

Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H																	He
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg											A*l*	Si	P	S	C*l*	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	T*l*	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac															

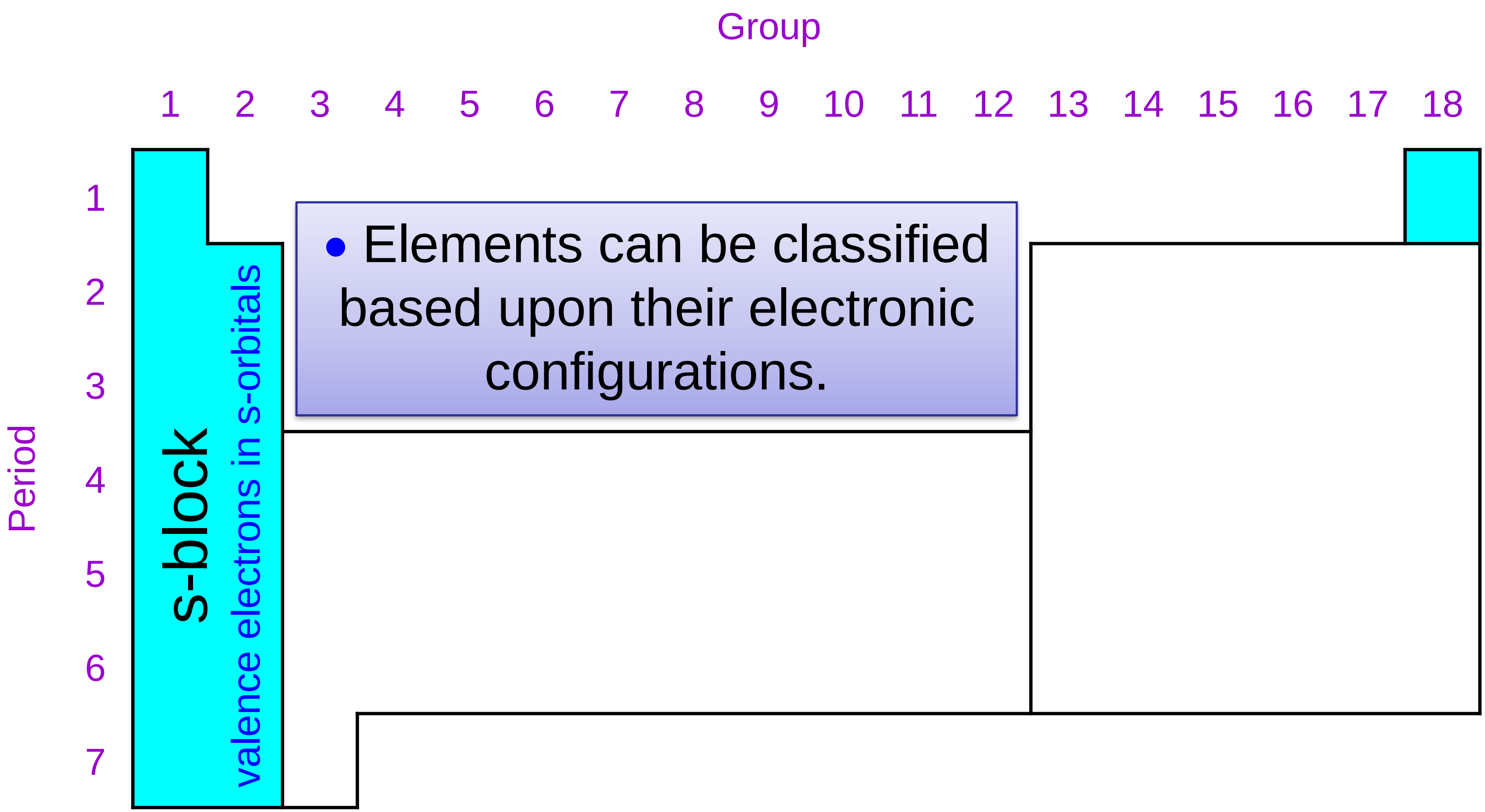
Advanced Theories of Atomic Structure

- Elements can be classified based upon their electronic configurations.

Group

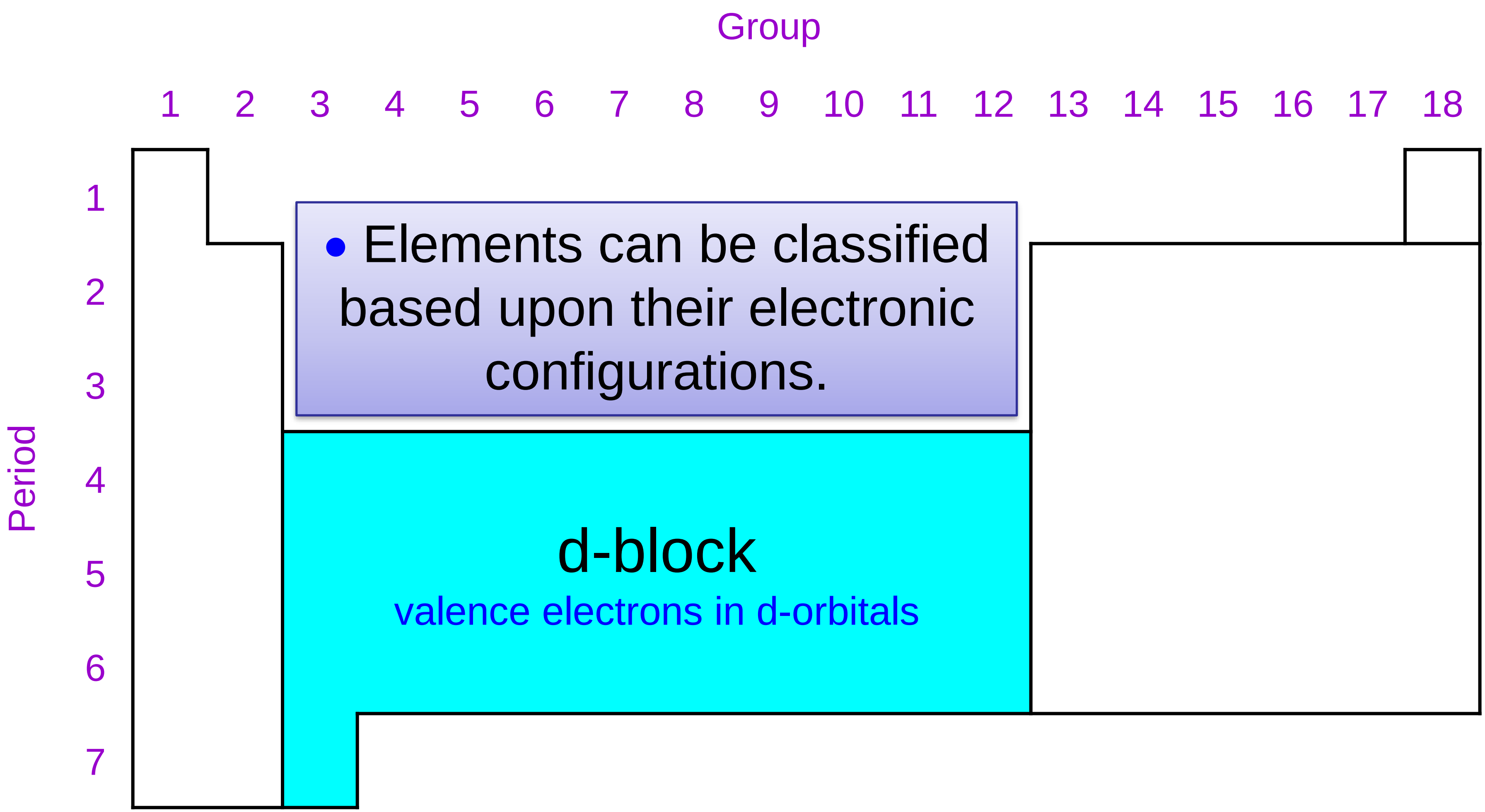
Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1s																	1s
2	2s	2s											2p	2p	2p	2p	2p	2p
3	3s	3s											3p	3p	3p	3p	3p	3p
4	4s	4s	3d	3d	3d	3d	3d	3d	3d	3d	3d	3d	4p	4p	4p	4p	4p	4p
5	5s	5s	4d	4d	4d	4d	4d	4d	4d	4d	4d	4d	5p	5p	5p	5p	5p	5p
6	6s	6s	5d	5d	5d	5d	5d	5d	5d	5d	5d	5d	6p	6p	6p	6p	6p	6p
7	7s	7s	6d															

Advanced Theories of Atomic Structure



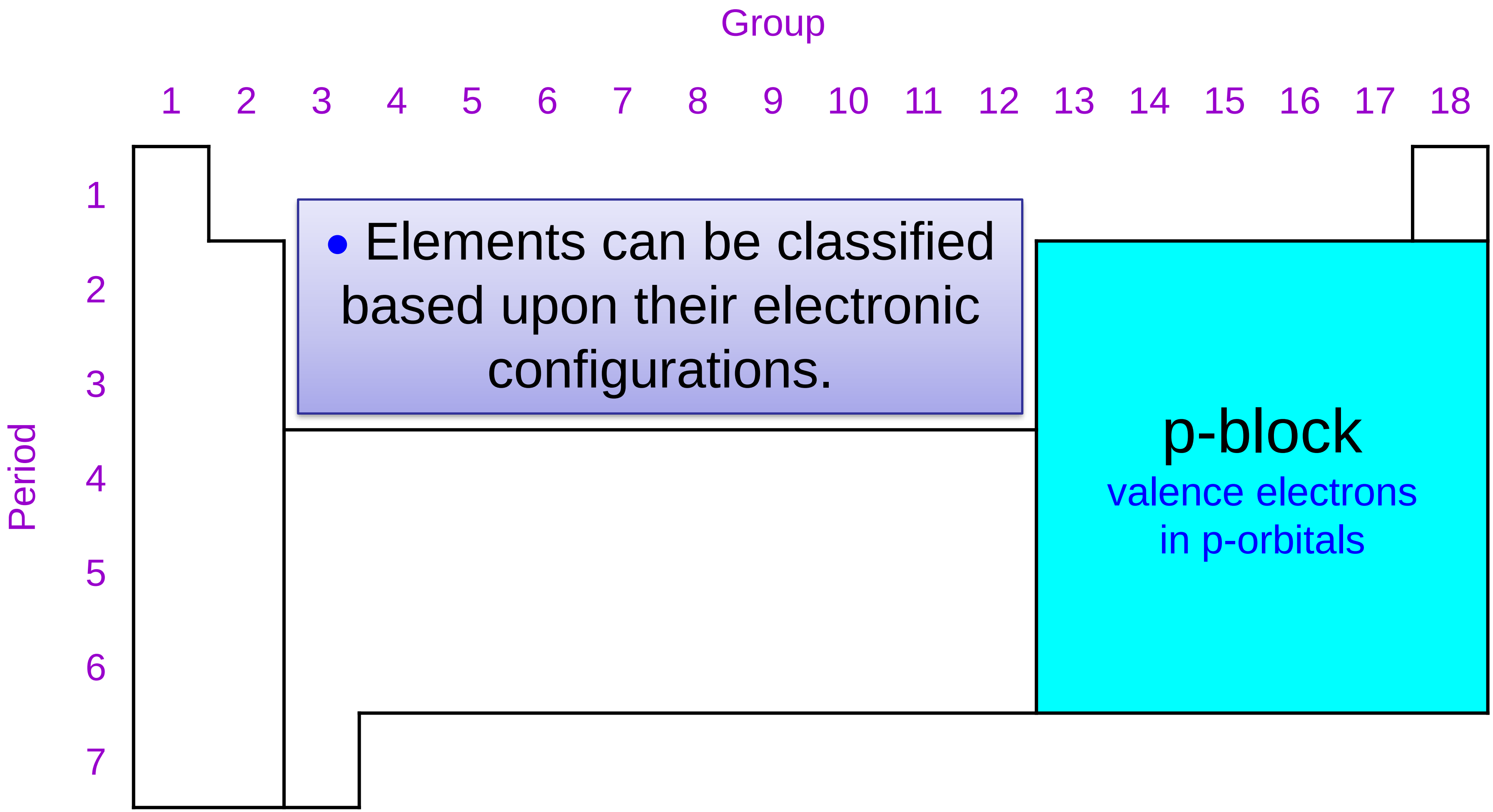
- Elements can be classified based upon their electronic configurations.

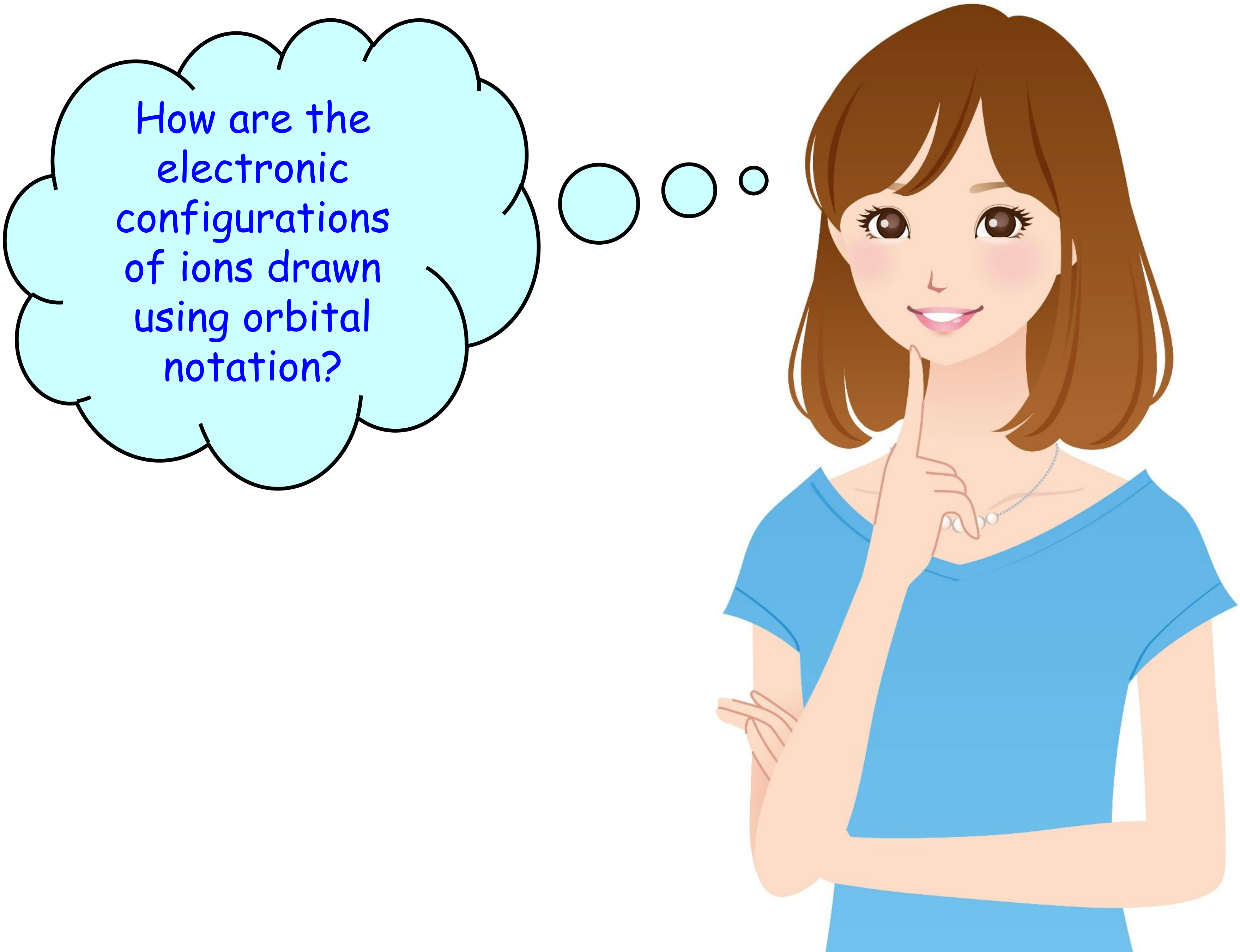
Advanced Theories of Atomic Structure



Advanced Theories of Atomic Structure

- Elements can be classified based upon their electronic configurations.

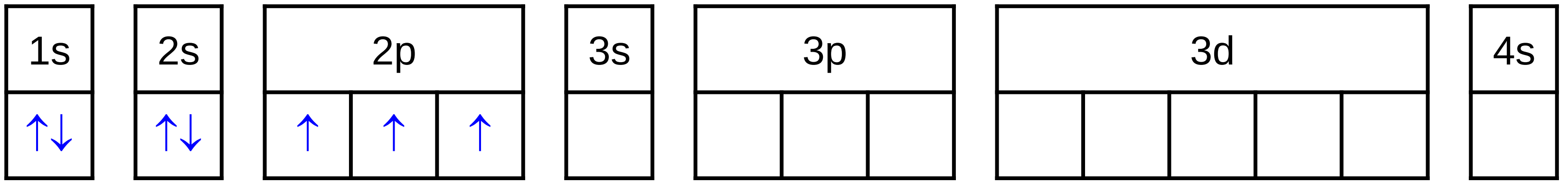



How are the electronic configurations of ions drawn using orbital notation?

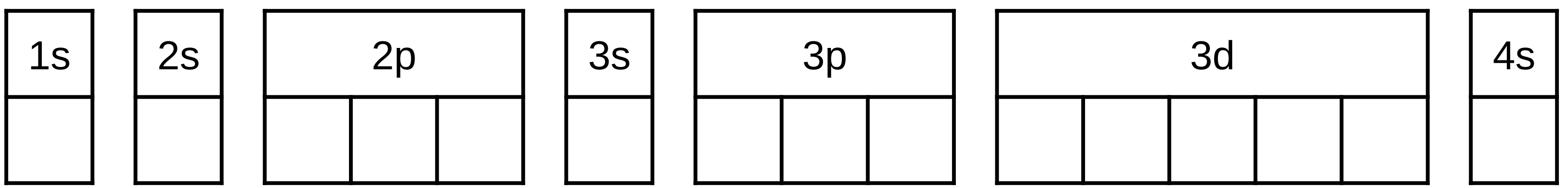
Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Nitrogen Atom



Electronic Configuration of a Nitride Ion – N^{3-}



Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Nitrogen Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑	↑	↑										

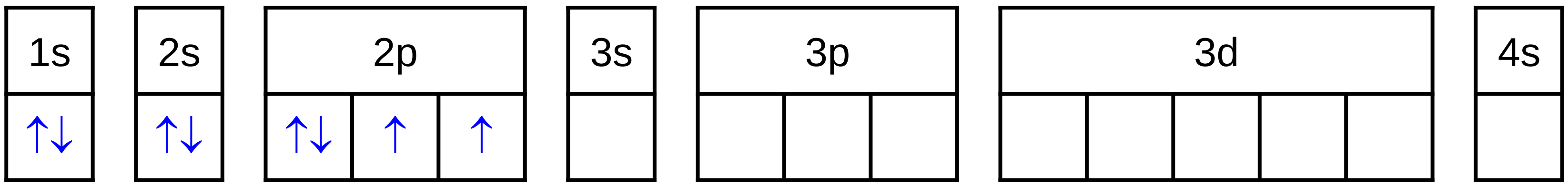
Electronic Configuration of a Nitride Ion – N^{3-}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓										

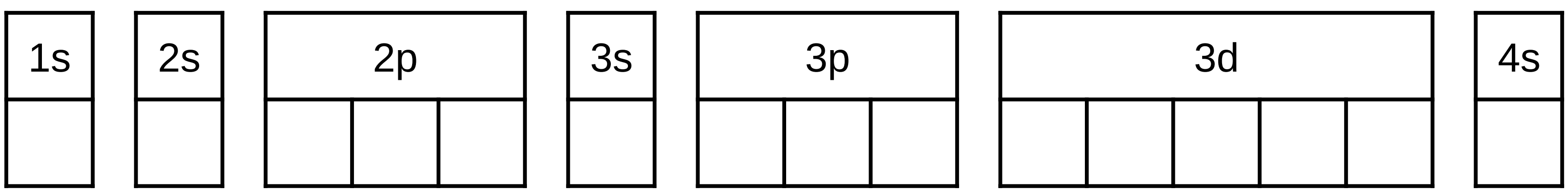
Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of an Oxygen Atom



Electronic Configuration of a Oxide Ion – O^{2-}



Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of an Oxygen Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑	↑										

Electronic Configuration of a Oxide Ion – O^{2-}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓										

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Chlorine Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑						

Electronic Configuration of a Chloride Ion – Cl^{-}

1s	2s	2p			3s	3p			3d					4s

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Chlorine Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑						

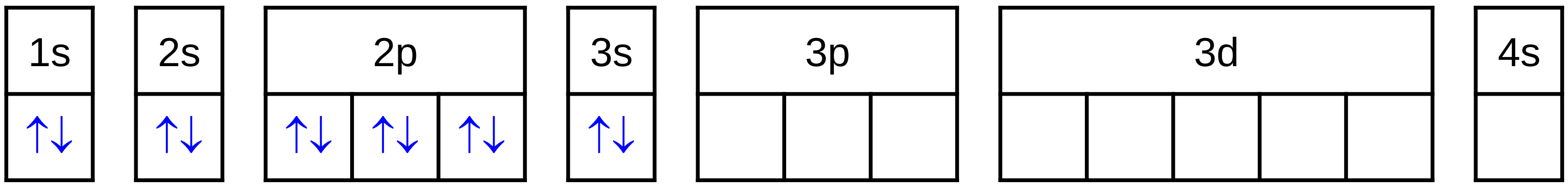
Electronic Configuration of a Chloride Ion – C*l*$^{-}$

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓						

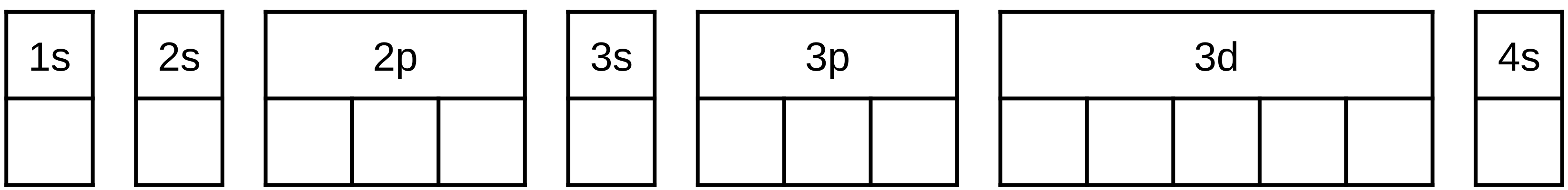
Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Magnesium Atom



Electronic Configuration of a Magnesium Ion – Mg^{2+}



Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Magnesium Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓									

Electronic Configuration of a Magnesium Ion – Mg^{2+}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓										

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of an Aluminium Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑								

Electronic Configuration of a Aluminium Ion – Al^{3+}

1s	2s	2p			3s	3p			3d					4s

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of an Aluminium Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑								

Electronic Configuration of a Aluminium Ion – Al^{3+}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓										

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Titanium Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑				↑↓

Electronic Configuration of a Titanium(III) Ion – Ti^{3+}

1s	2s	2p			3s	3p			3d					4s

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Titanium Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑				↑↓

Electronic Configuration of a Titanium(III) Ion – Ti^{3+}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑					

Note: When atoms of the transition metals react to form ions, electrons from the 4s orbital are the first to be removed.

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Chromium Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑	↑

Electronic Configuration of a Chromium(III) Ion – Cr^{3+}

1s	2s	2p			3s	3p			3d					4s

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Chromium Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑	↑

Electronic Configuration of a Chromium(III) Ion – Cr^{3+}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑			

Note: When atoms of the transition metals react to form ions, electrons from the 4s orbital are the first to be removed.

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of an Iron Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑↓

Electronic Configuration of a Iron(II) Ion – Fe^{2+}

1s	2s	2p			3s	3p			3d					4s

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of an Iron Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑↓

Electronic Configuration of a Iron(II) Ion – Fe^{2+}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	

Note: When atoms of the transition metals react to form ions, electrons from the 4s orbital are the first to be removed.

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of an Iron Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑↓

Electronic Configuration of a Iron(III) Ion – Fe^{3+}

1s	2s	2p			3s	3p			3d					4s

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of an Iron Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑↓

Electronic Configuration of a Iron(III) Ion – Fe^{3+}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑	

Note: When atoms of the transition metals react to form ions, electrons from the 4s orbital are the first to be removed.

Note: In the iron(III) ion, the 3d orbital is half-full, and therefore stable.

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Copper Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑

Electronic Configuration of a Copper(II) Ion – Cu^{2+}

1s	2s	2p			3s	3p			3d					4s

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Copper Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑

Electronic Configuration of a Copper(II) Ion – Cu^{2+}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	

Note: When atoms of the transition metals react to form ions, electrons from the 4s orbital are the first to be removed.

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Zinc Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

Electronic Configuration of a Zinc Ion – Zn^{2+}

1s	2s	2p			3s	3p			3d					4s

Advanced Theories of Atomic Structure

Electronic Configurations of Ions

Electronic Configuration of a Zinc Atom

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

Electronic Configuration of a Zinc Ion – Zn^{2+}

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	

Note: When atoms of the transition metals react to form ions, electrons from the 4s orbital are the first to be removed.


What is Valence Bond Theory?

Advanced Theories of Atomic Structure

Valence Bond Theory

- *Valence bond theory* describes a covalent bond as the overlap of half-filled atomic orbitals (each containing a single electron) that produce a pair of electrons shared between the two bonded atoms. Orbitals on two different atoms *overlap* when a portion of one orbital and a portion of a second orbital occupy the *same region of space*.

- According to valence bond theory, a covalent bond results when two conditions are met:

1. An orbital on one atom overlaps an orbital on a second atom.

2. The single electrons in each orbital combine to form an electron pair.

Advanced Theories of Atomic Structure

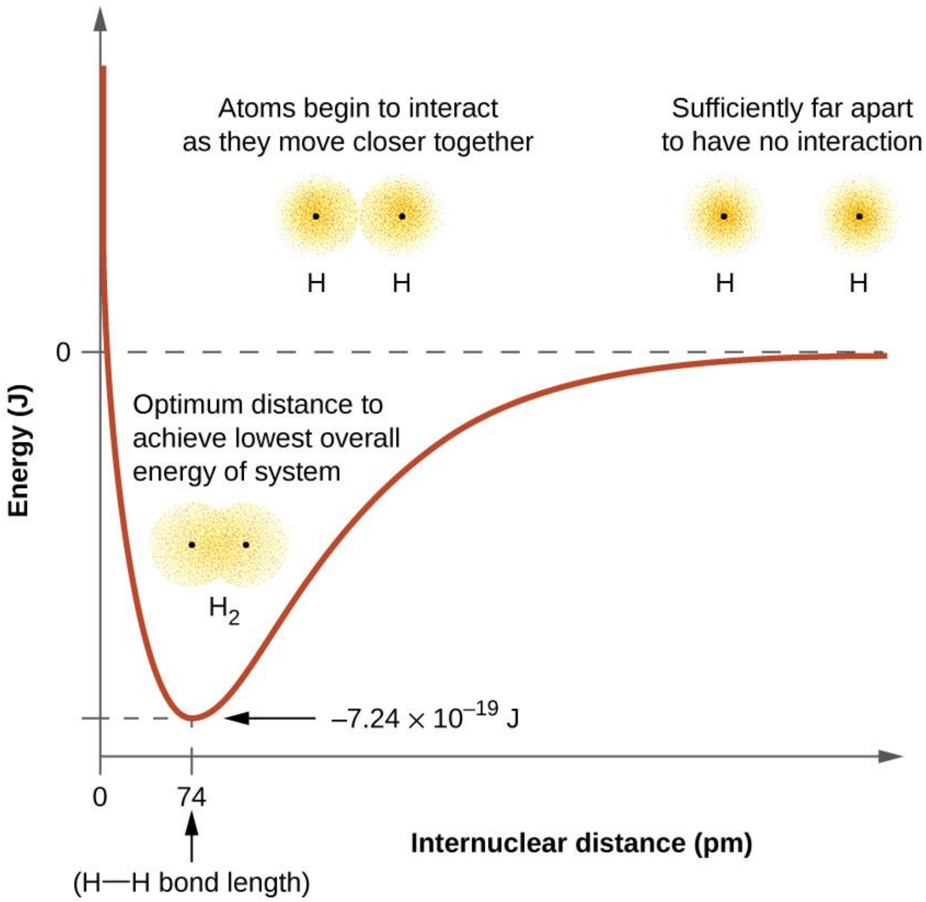
Valence Bond Theory

- The electrostatic force of attraction between the negatively charged pair of electrons and the positively charged nuclei of the two atoms that are sharing them serves to physically link the two atoms together through a force we define as a *covalent bond*.

- The strength of a covalent bond depends on the extent of overlap of the orbitals involved. Orbitals that overlap extensively form bonds that are stronger than those that have less overlap.

Advanced Theories of Atomic Structure

Valence Bond Theory



- This diagram illustrates how the atomic orbitals of two hydrogen atoms interact. At a *large separation*, there is *no interaction* between the atomic orbitals. At a *very small separation*, the atoms *repel* each other. The two atoms are at their *lowest energy*, *i.e.* *most stable*, at a distance of 7.4×10^{-11} m, which is the H–H *covalent bond length*.

How is bonding between atoms represented using orbital notation?

Advanced Theories of Atomic Structure

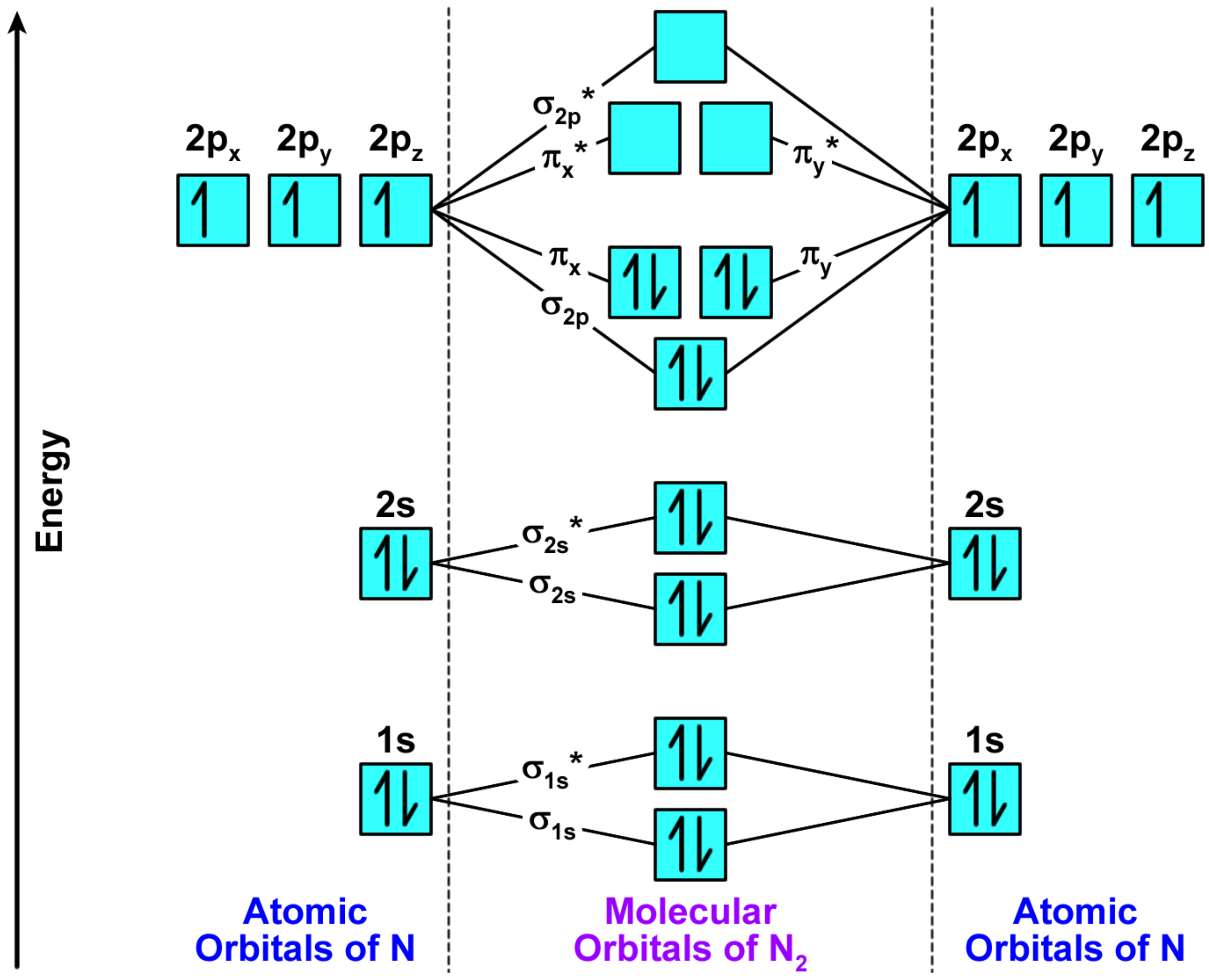
- The *atomic orbitals* of two or more atoms can combine together to form *molecular orbitals*.

- The following diagrams show how the atomic orbitals of two atoms combine to form covalent bonds known as a σ-bonds (sigma-bonds) and π-bonds (pi-bonds).

- **Note:** To pair-up in a molecular orbital, electrons must have *opposite spin*.

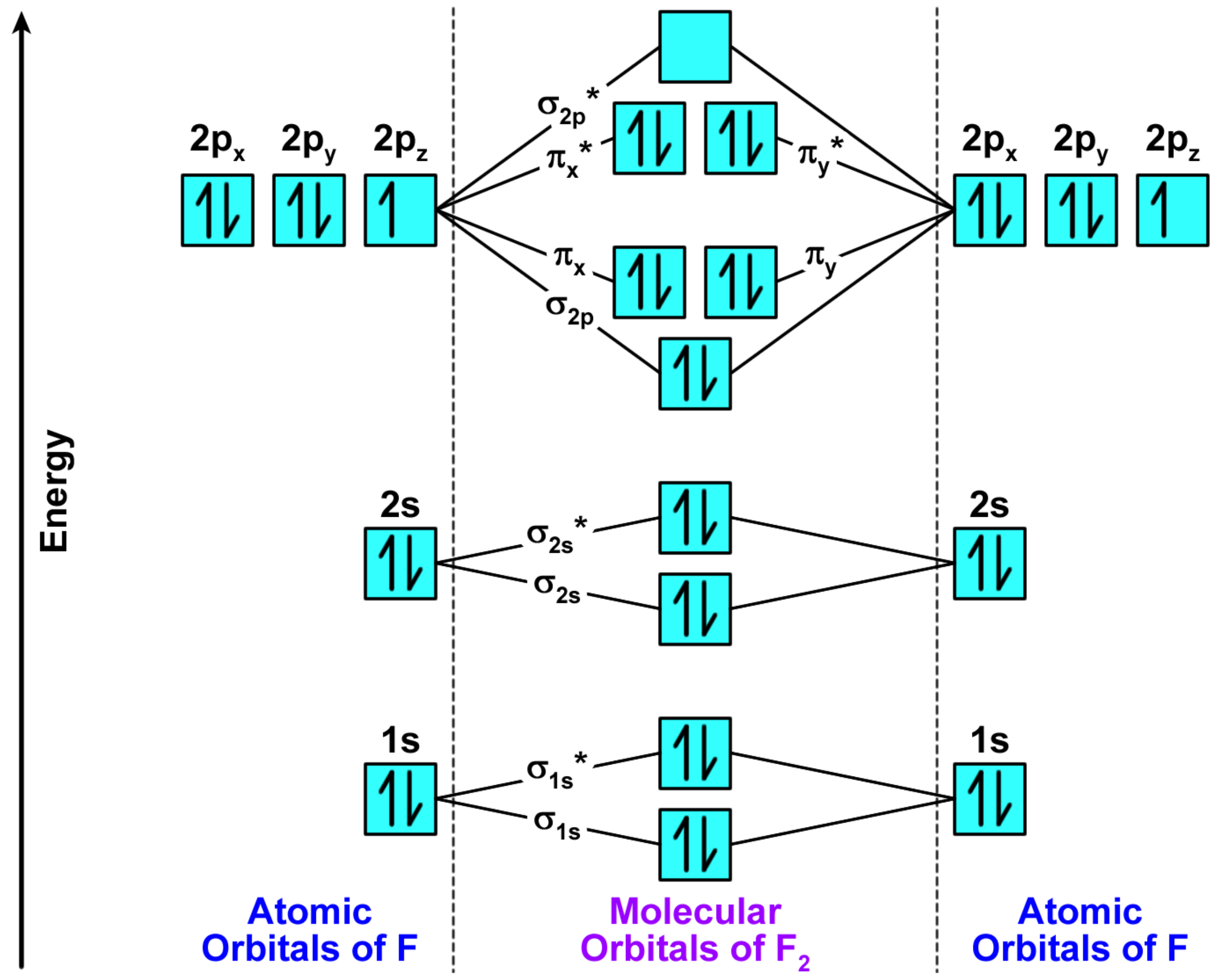
Advanced Theories of Atomic Structure

The Molecular Orbitals in Diatomic Nitrogen – N_2



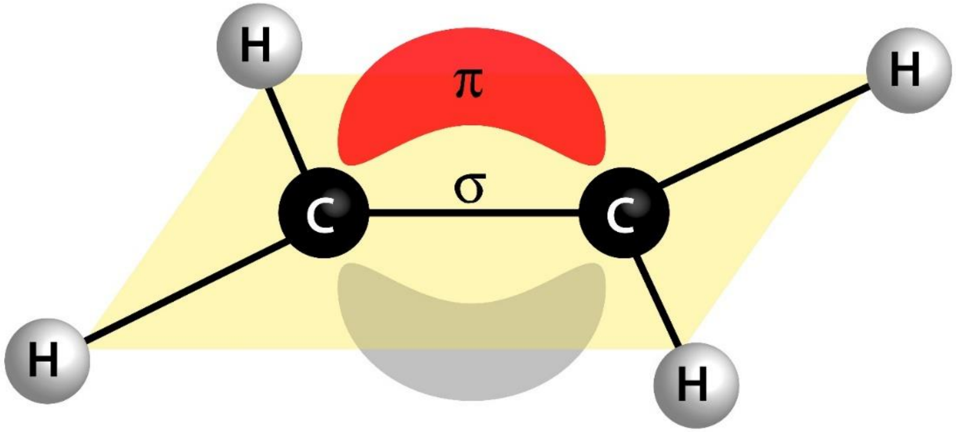
Advanced Theories of Atomic Structure

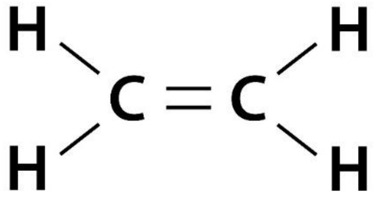
The Molecular Orbitals in Diatomic Fluorine – F_2



Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

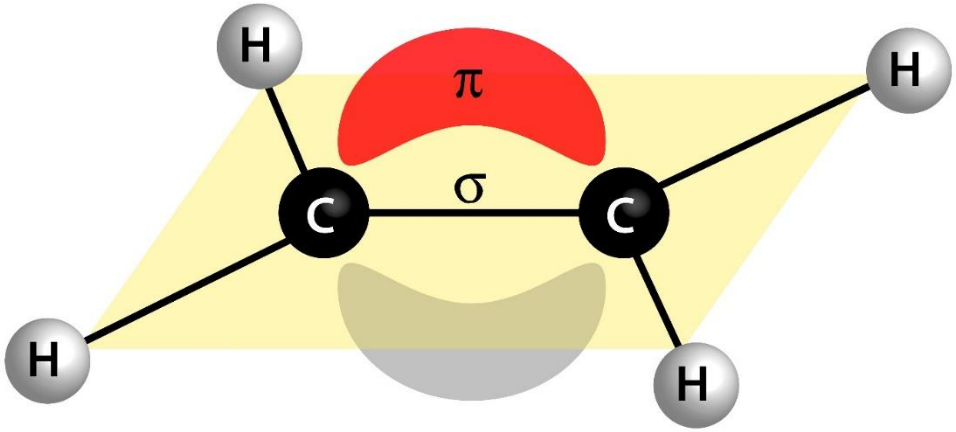


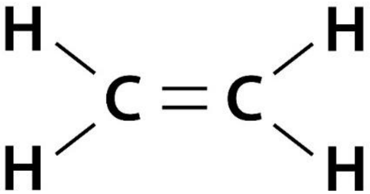


- Examples of *σ-bonds* and *π-bonds* in a molecule of ethene, C_2H_4.

Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

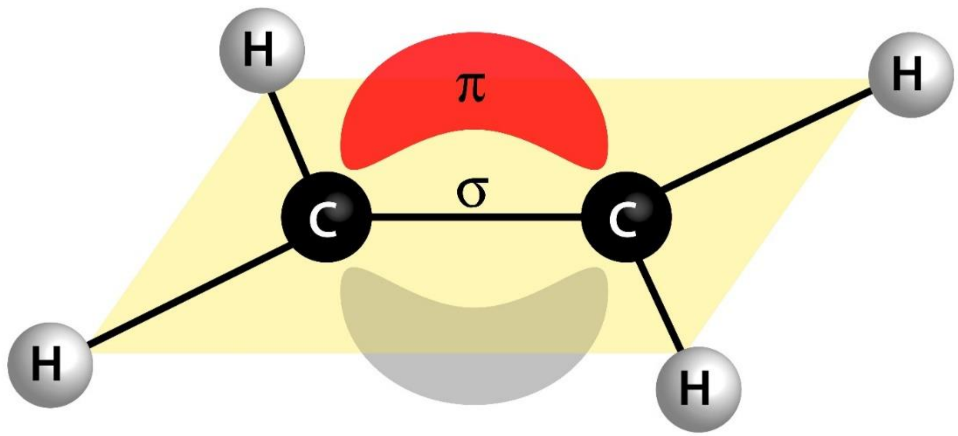


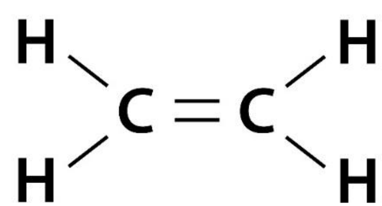


• A *σ-bond* is formed when two atomic orbitals overlap, and the region of overlap (region of highest electron density) lies on an imaginary straight line that connects the nuclei of the two bonding atoms.

Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

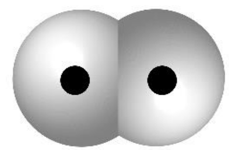




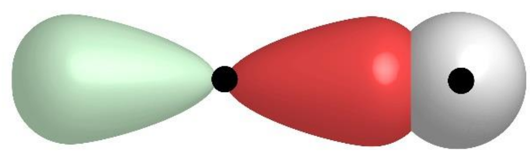
- A *π-bond* is formed when two atomic orbitals (usually *p*-orbitals) overlap, and the region of overlap (region of highest electron density) lies above and below an imaginary straight line that connects the nuclei of the two bonding atoms.

Advanced Theories of Atomic Structure

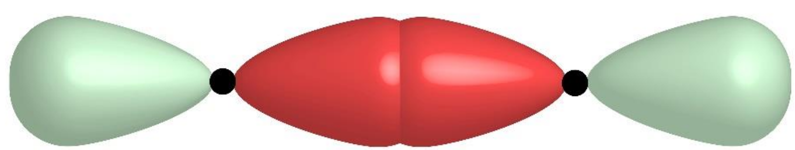
Pi-Bonds and Sigma-Bonds



$\sigma_{s\text{–}s}$



$\sigma_{p\text{–}s}$

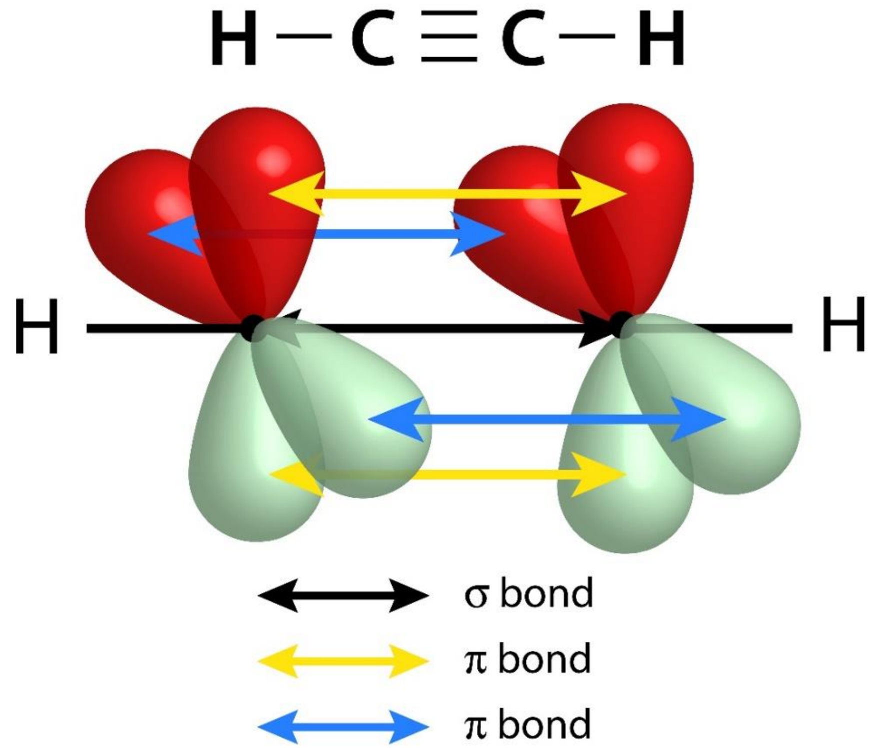


$\sigma_{p\text{–}p}$

- Different ways of forming *σ-bonds*. Note that the region of orbital overlap (region of highest electron density) is directly in-between the nuclei of the two bonding atoms.

Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds



- Bonding in a molecule of ethyne, C_2H_2. The two carbon atoms are bonded together by *one σ-bond* and *two π-bonds*. A single σ-bond joins each carbon to hydrogen.

Advanced Theories of Atomic Structure

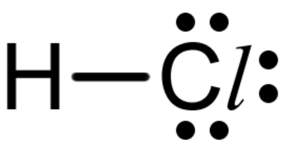
Pi-Bonds and Sigma-Bonds

- Two atoms can be held together by a maximum number of *one σ-bond*, but by *one or more π-bonds*.
- σ-bonds are *always* formed between two atoms *before* any π-bonds are formed.
- How many *σ-bonds* and how many *π-bonds* are there in each one of the molecules shown below?

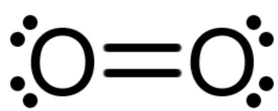
Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

- Two atoms can be held together by a maximum number of *one σ-bond*, but by *one or more π-bonds*.
- σ-bonds are *always* formed between two atoms *before* any π-bonds are formed.
- How many *σ-bonds* and how many *π-bonds* are there in each one of the molecules shown below?

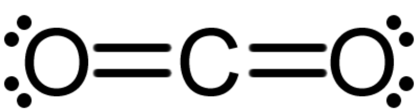


1 σ-bond
0 π-bonds



1 σ-bond
1 π-bond

1 σ-bond
2 π-bonds

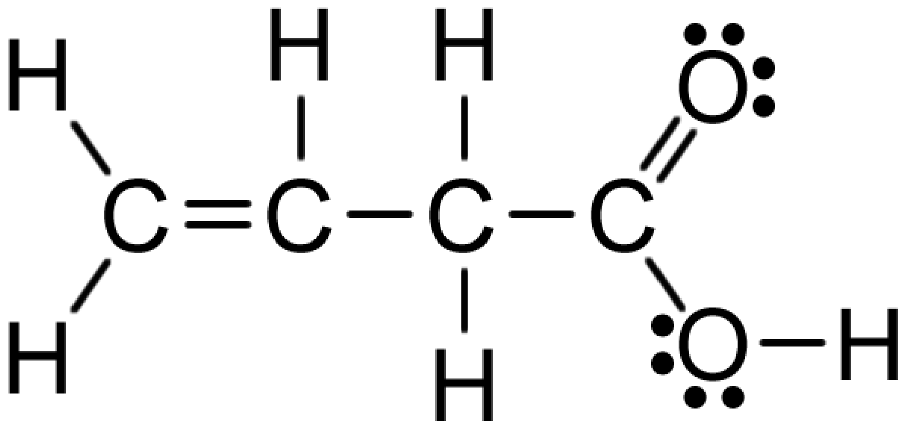


2 σ-bonds
2 π-bonds

Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

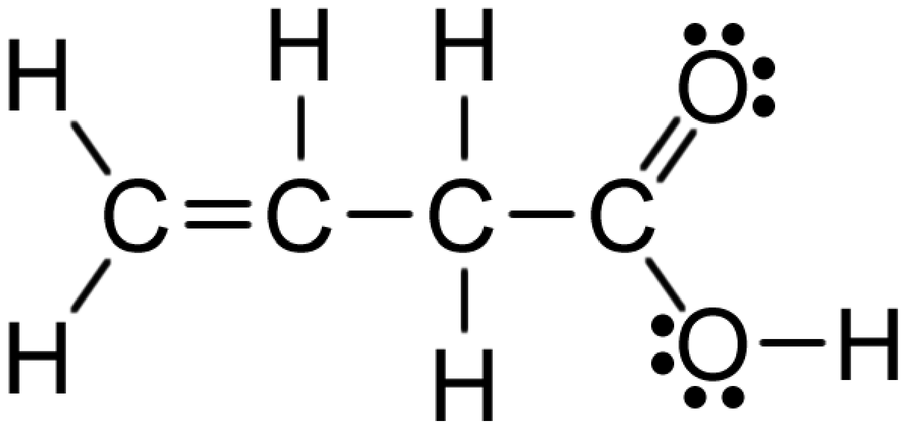
- How many *σ-bonds* and how many *π-bonds* are there in the molecule shown below?



Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

- How many *σ-bonds* and how many *π-bonds* are there in the molecule shown below?



- There are 13 covalent bonds in total:

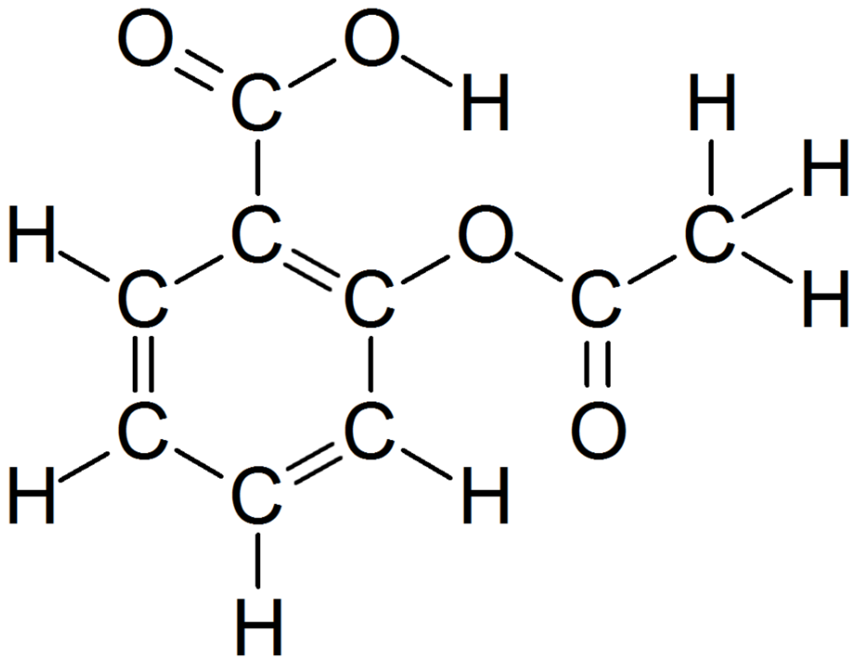
  11 σ-bonds

  2 π-bonds

Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

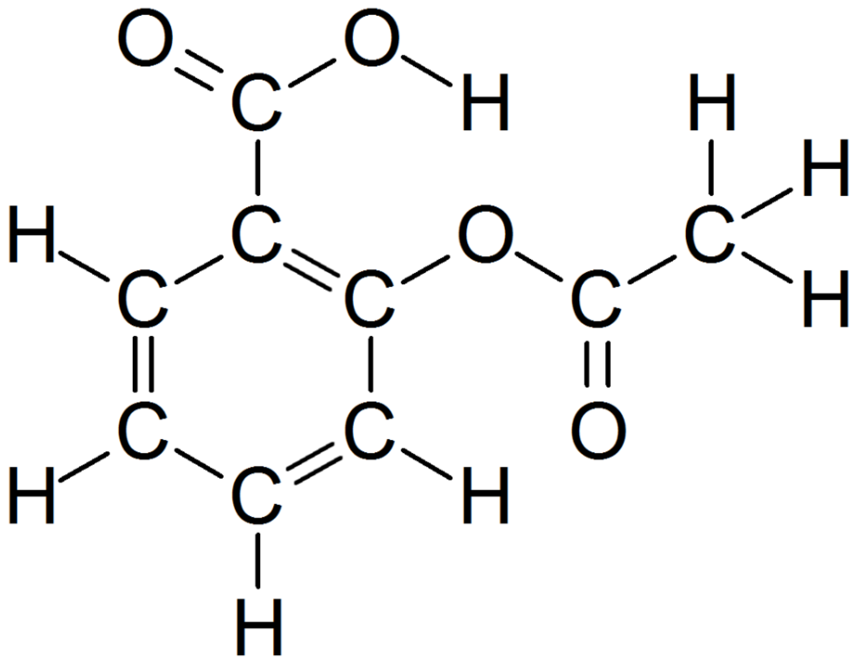
- How many *σ-bonds* and how many *π-bonds* are there in the molecule of *aspirin* shown below?



Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

- How many *σ-bonds* and how many *π-bonds* are there in the molecule of *aspirin* shown below?



- There are 26 covalent bonds: 21 σ-bonds and 5 π-bonds

Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

- Is a carbon-to-carbon *double* covalent bond (one σ-bond and one π-bond) *twice the strength* of a carbon-to-carbon *single* covalent bond (one σ-bond)?

- C=C bond energy = 602 kJ/mol

- C–C bond energy = 346 kJ/mol

Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

- Is a carbon-to-carbon *double* covalent bond (one σ-bond and one π-bond) *twice the strength* of a carbon-to-carbon *single* covalent bond (one σ-bond)?

- C=C bond energy = 602 kJ/mol

- C–C bond energy = 346 kJ/mol

- $602 \div 2 = 301$ kJ/mol and $301 < 346$

OR

- $346 \times 2 = 692$ kJ/mol and $692 > 602$

$\therefore$ A C=C bond is *less* than twice the strength of a C–C bond.

Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

- C=C bonds are less than twice the strength of C–C bonds, illustrating that π-bonds are weaker then σ-bonds.

- The strength of a σ-bond is 346 kJ/mol
- The strength of a π-bond is 602 – 346 = 256 kJ/mol

- For *σ-bonds*, the region of orbital overlap is directly between the nuclei of the two bonding atoms. The volume of orbital overlap is *relatively large*, and hence the *electrostatic forces of attraction are relatively strong, and a large amount of energy is required to break the σ-bond*.

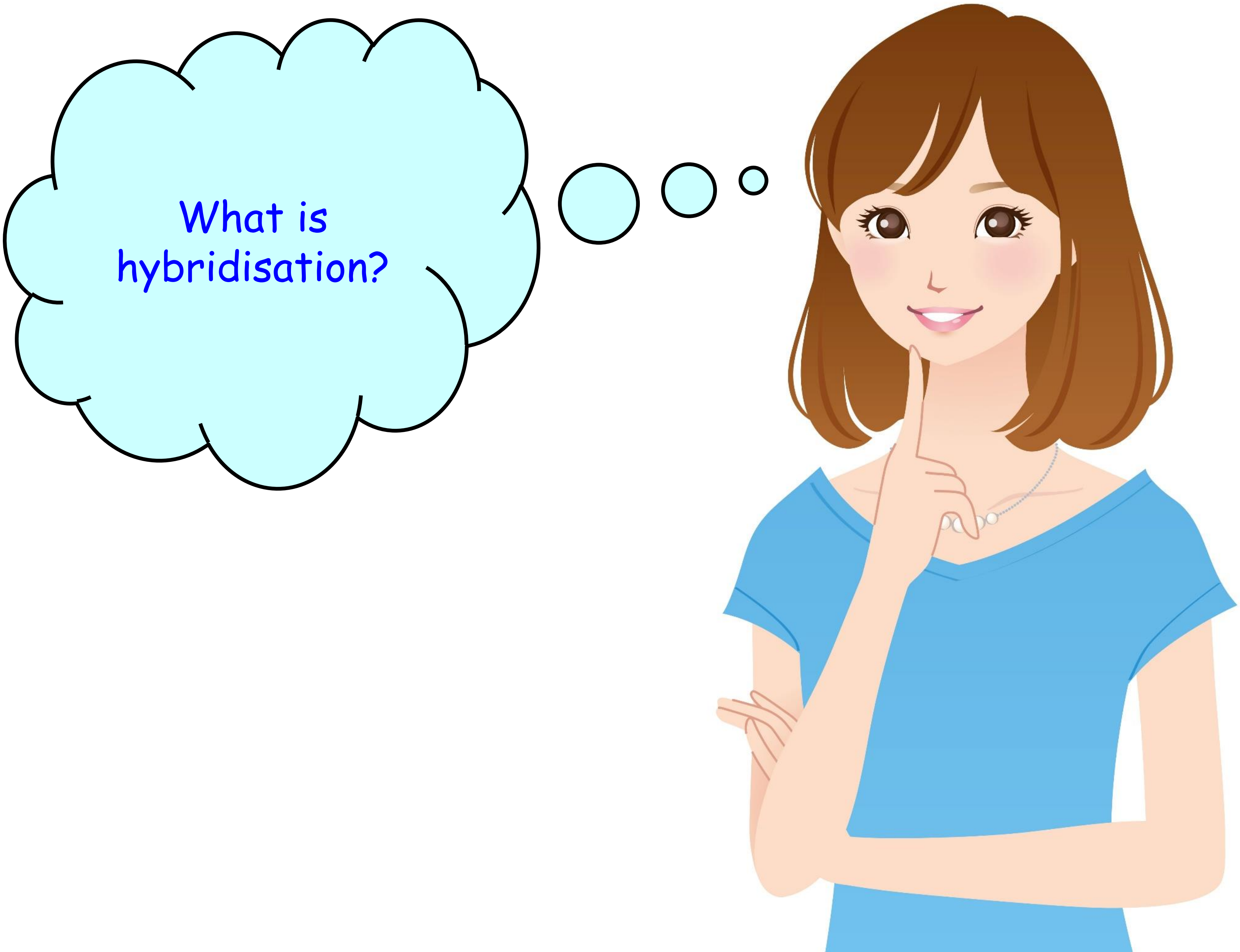
Advanced Theories of Atomic Structure

Pi-Bonds and Sigma-Bonds

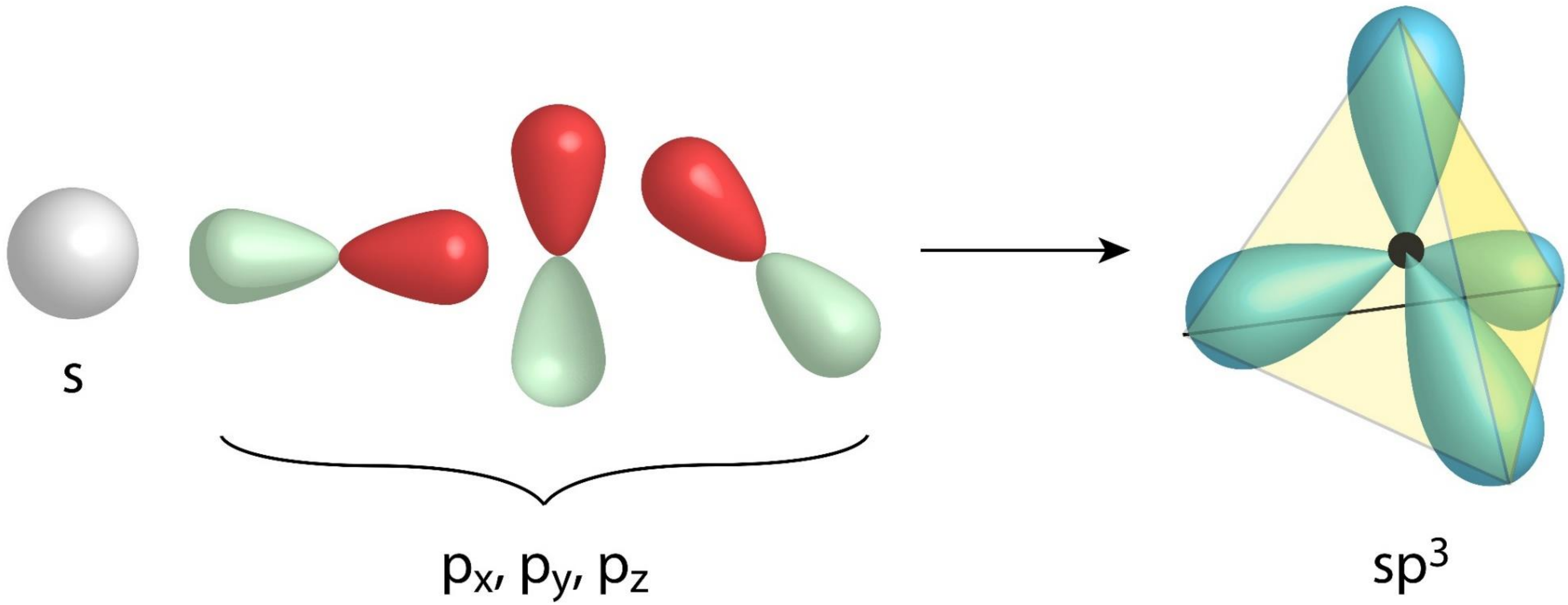
- C=C bonds are less than twice the strength of C–C bonds, illustrating that π-bonds are weaker then σ-bonds.

- The strength of a σ-bond is 346 kJ/mol
- The strength of a π-bond is 602 – 346 = 256 kJ/mol

- For *π-bonds*, the region of orbital overlap is not directly between the nuclei of the two bonding atoms. The volume of orbital overlap is *relatively small*, and hence the *electrostatic forces of attraction are relatively weak, and only a small amount of energy is required to break the π-bond*.

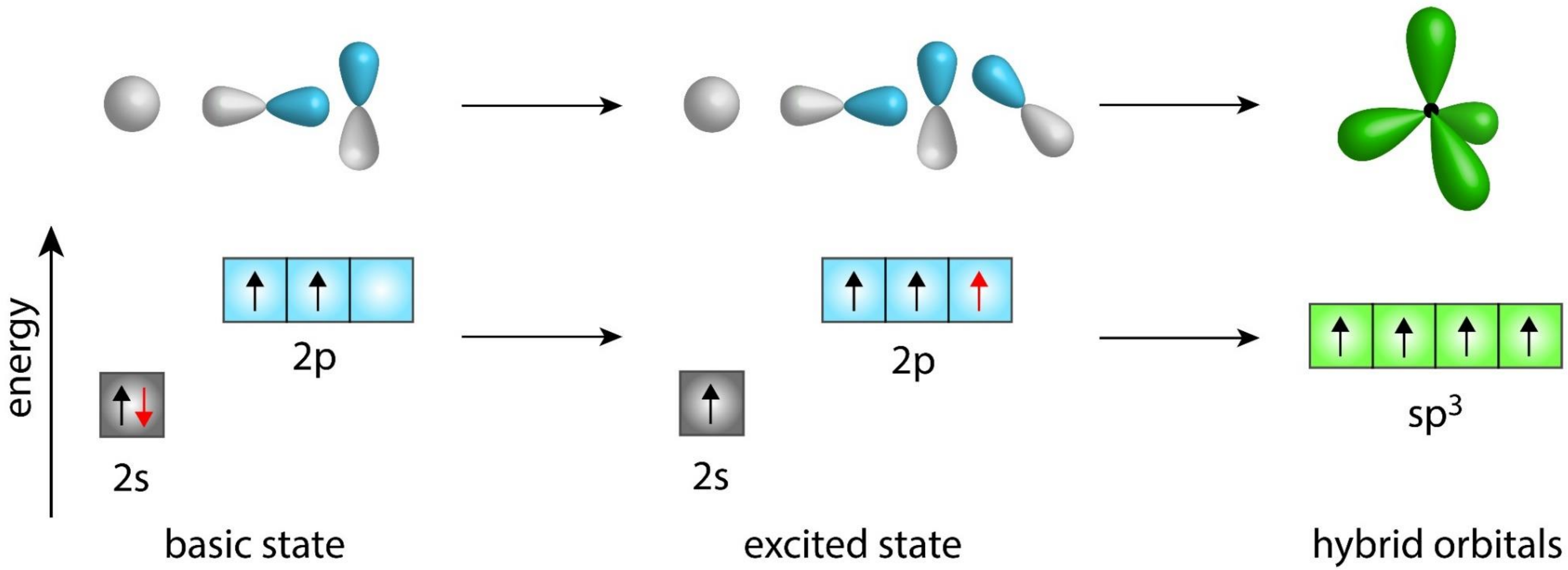

What is
hybridisation?

Advanced Theories of Atomic Structure



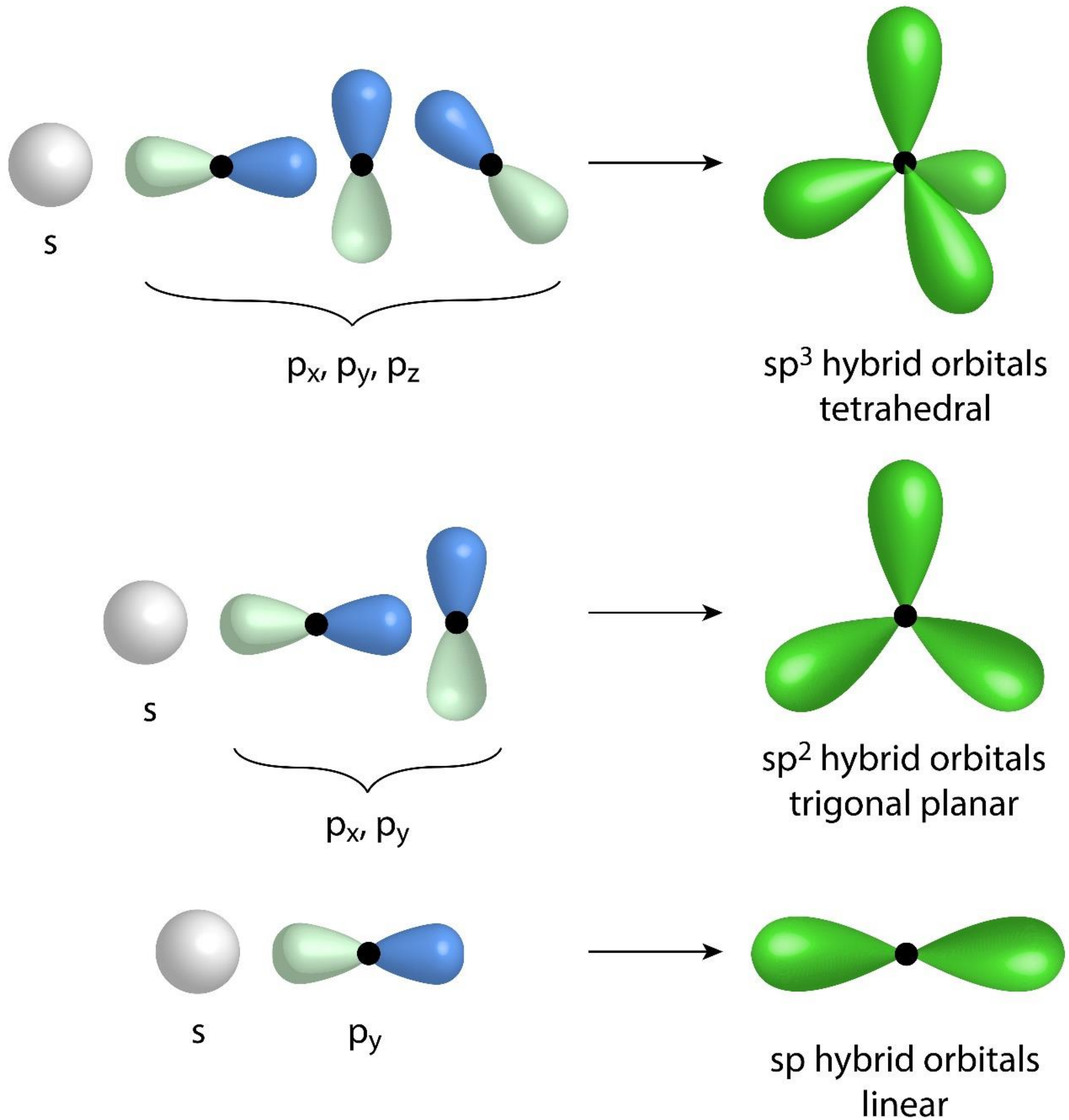
- In chemistry, *hybridisation* is the concept of combining atomic orbitals to form new *hybrid* orbitals that have different shapes and energies compared to the original atomic orbitals.

Advanced Theories of Atomic Structure



- Once hybridisation of atomic orbitals has occurred, electrons in the new hybrid orbitals can be shared with other atoms to form *covalent bonds*. Hybridisation is very useful in explaining the *molecular geometry* or shapes of certain molecules, *e.g.* the *tetrahedral* shape of methane – CH_4.

Advanced Theories of Atomic Structure




What are some periodic trends that can be explained using orbital theory?

Periodic Trends

- The force of attraction between oppositely charged particles is given by Coulomb's Law:

$$F = \frac{1}{4 \times \pi \times \varepsilon_0} \times \frac{q_1 \times q_2}{r^2}$$

F = force of attraction between oppositely charged particles, N

ε_0 = permittivity of free space, $C^2\ m^{-2}\ N^{-1}$

q_1 = charge on particle one, C

q_2 = charge on particle two, C

r = distance between particle one and particle two, m

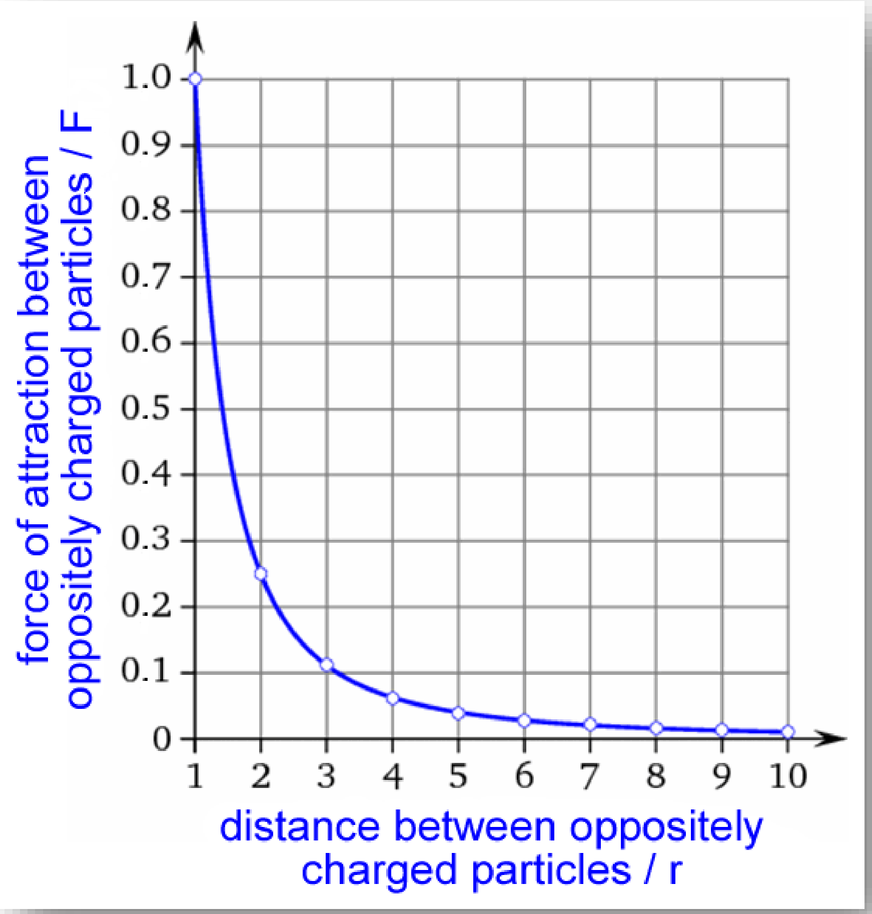
Periodic Trends

- The force of attraction between oppositely charged particles is given by Coulomb's Law:

$$F \propto \frac{q_1 \times q_2}{r^2}$$

- The *force of attraction* (F) between a proton and an electron in an atom is related to their *charge* (q_1 and q_2), and it *decreases rapidly* as the *distance* between the particles (r) *increases* (inverse square law).

Periodic Trends

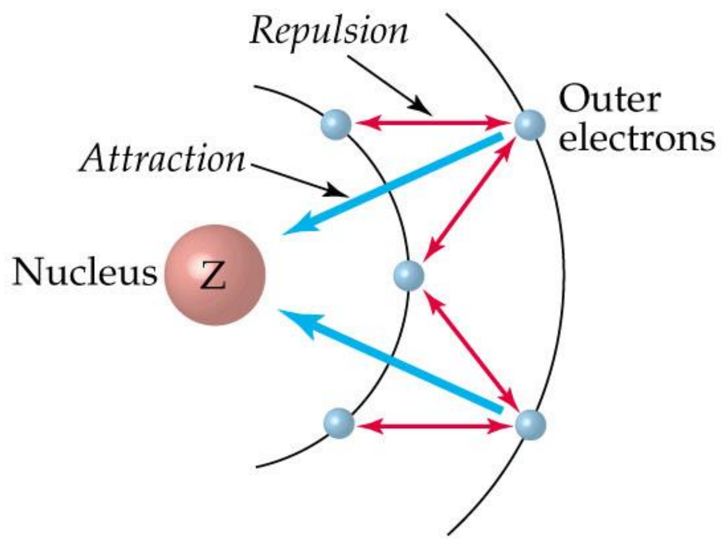


- The force of attraction (F) between two oppositely charged particles decreases rapidly as the distance between the particles (r) increases – inverse square law.

Periodic Trends

- A note about *effective nuclear charge*.

- In an atom with many electrons, the negatively charged electron(s) in the *valence shell* is simultaneously *attracted* towards the positively charged nucleus and *repelled* by the negatively charged electrons of the inner electron shells.



Periodic Trends

- A note about *effective nuclear charge*.

- The *effective nuclear charge* is the overall charge that an electron(s) in the valence shell of an atom experiences. This takes into account:

→ The number of positively charged protons in the nucleus of the atom (atomic number) that are *attracting* the negatively charged valence electron(s).

→ The number of negatively charged electrons occupying the inner electron shells that are *repelling* the negatively charged valence electron(s). This is often referred to as the *shielding effect*, as these electrons *shield* the valence electron(s) from attractive force of the positively charged nucleus.

Periodic Trends

- A note about *effective nuclear charge*.

$$Z_{\text{eff}} = Z - S$$

Where:

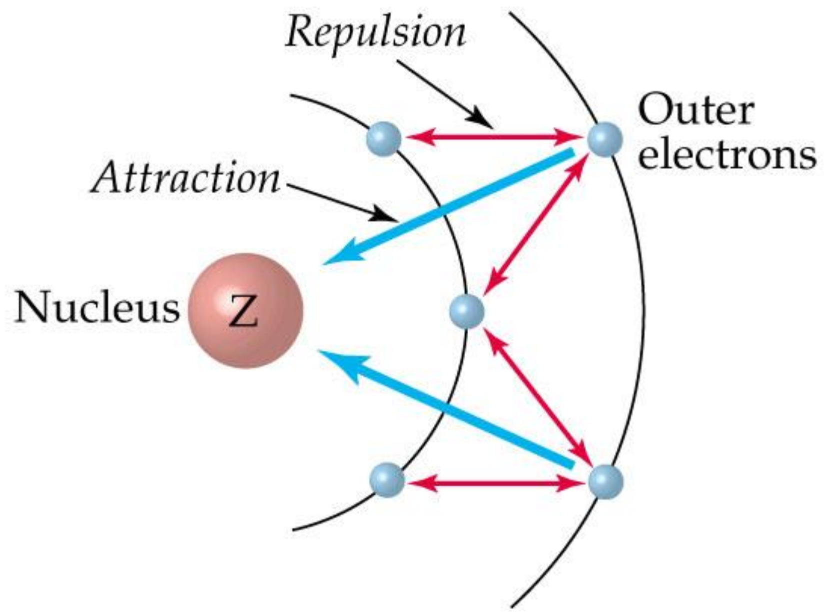
Z_{eff} = the effective nuclear charge.

Z = the number of positively charged protons in the nucleus of the atom (atomic number).

S = the number of electrons in-between the positively charged nucleus and negatively charged valence electron(s), *i.e.* the number of non-valence electrons, which give rise to the *shielding effect*.

Periodic Trends

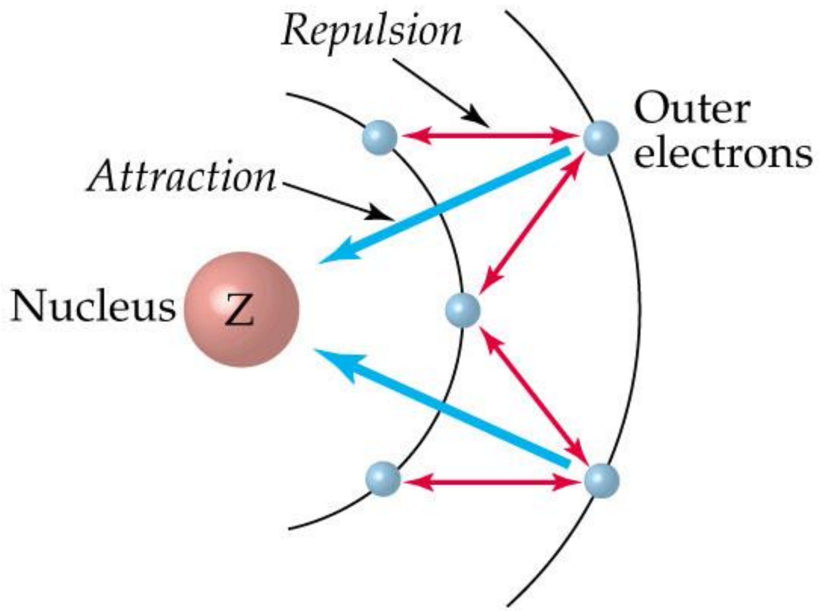
- A note about *shielding effect*.



- Electrons in the valence shell of the atom are *shielded* from the positively charged nucleus by negatively charged electrons of the inner electron shells. *Shielding* results in the valence electrons experiencing a *weaker effective nuclear charge*.

Periodic Trends

- A note about *shielding effect*.

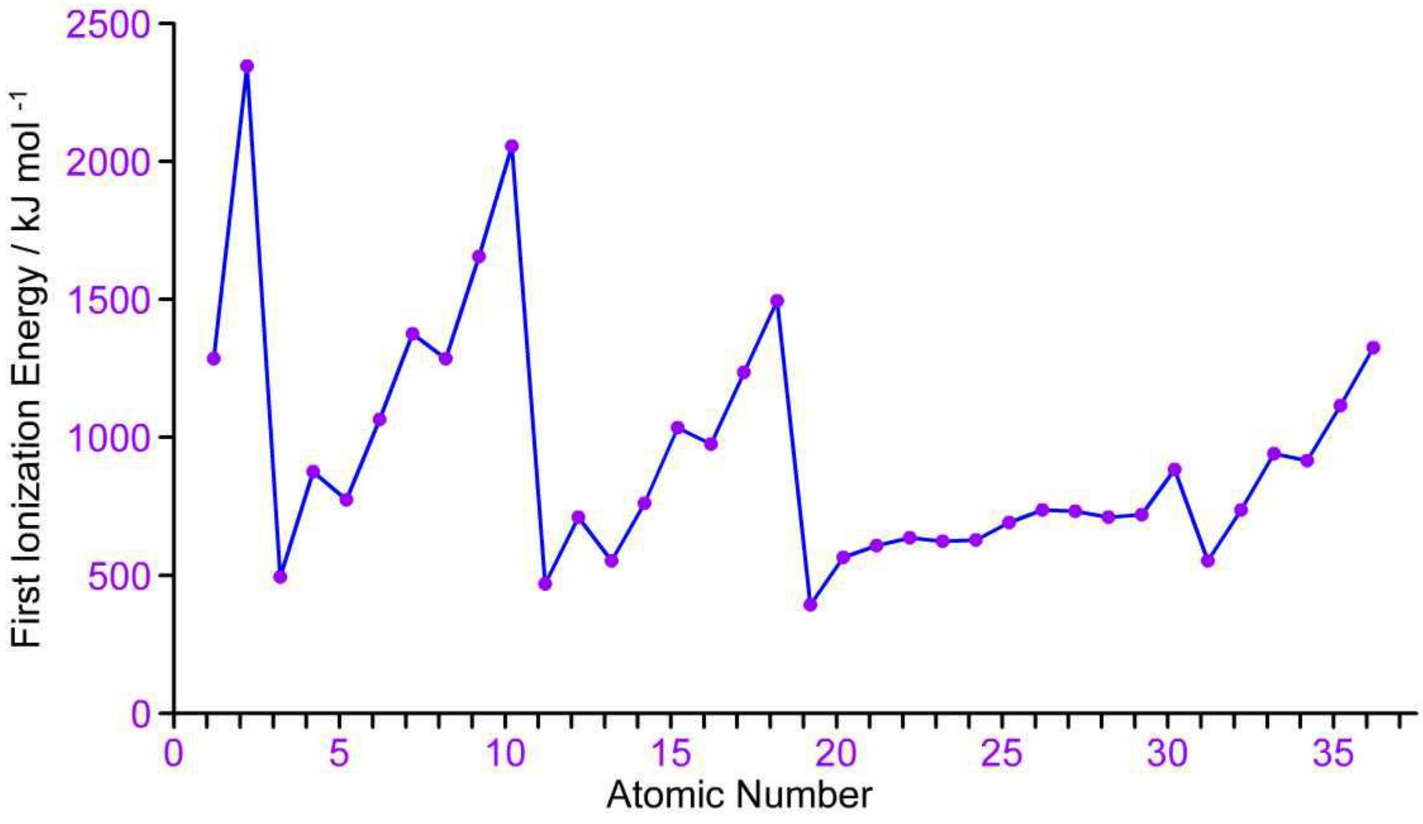


- Due to the *shielding effect*, the *electrostatic force of attraction* between the positively charged protons in the nucleus and negatively charged electron(s) in the valence shell of the atom is *reduced*.

Periodic Trends

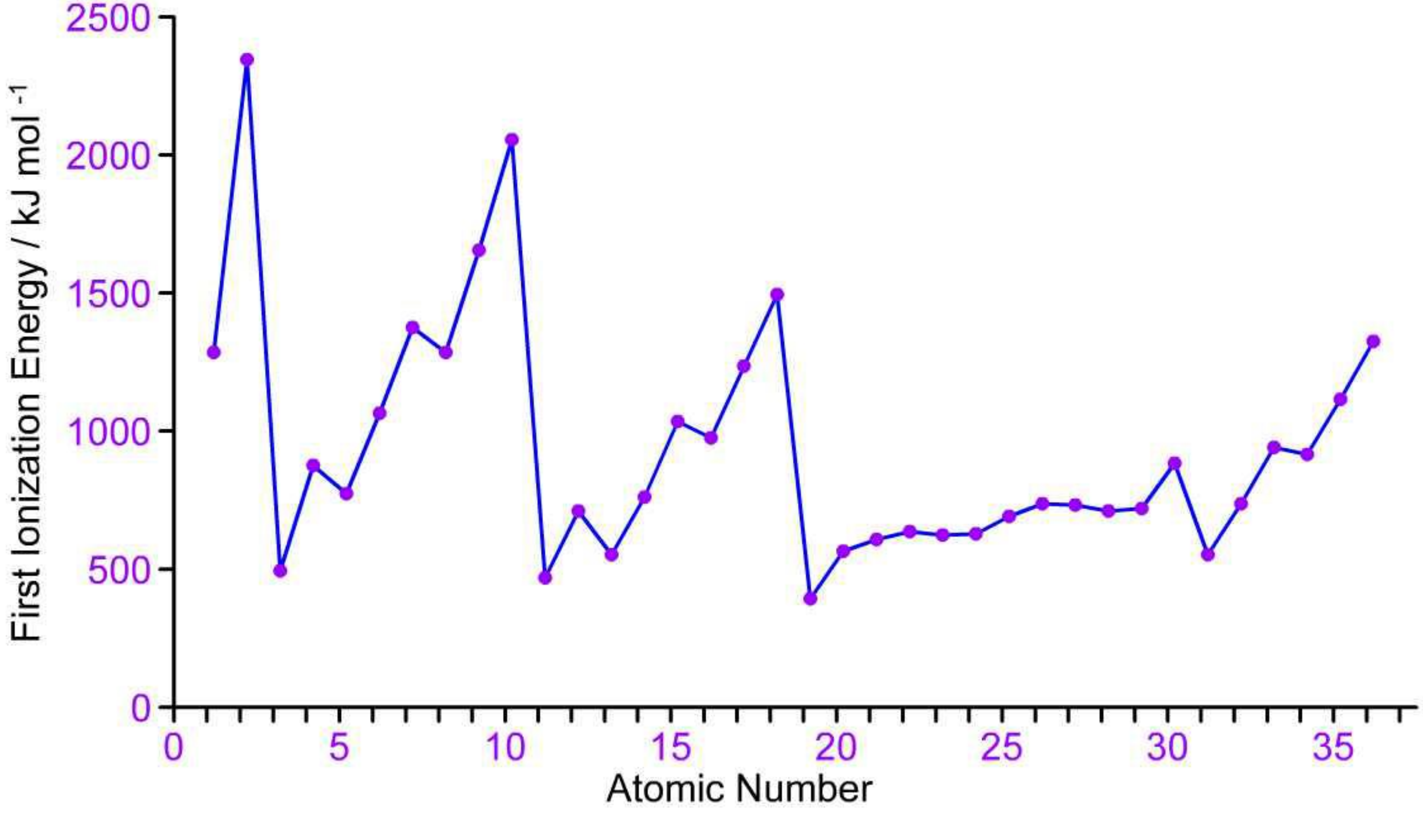
- First ionization energy is the energy required to convert 1 mole (6×10^{23}) of gaseous atoms into one mole (6×10^{23}) of unipositive (1+) gaseous ions.

$$E(g) \rightarrow E^{+}(g) + e^{-}$$



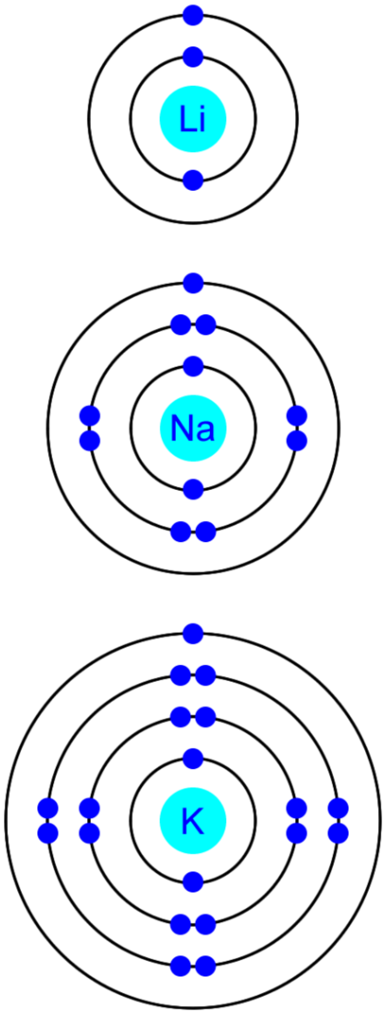
Periodic Trends

- Essentially, first ionization energy gives an indication of the amount of energy that is required to remove a single electron from the valence shell of a single atom.



Periodic Trends

- First ionization energy *decreases down a Group*.



- The number of protons in the nucleus of an atom (nuclear charge) and the number of electron shells around the nucleus of the atom *both increase* down a Group.

- Moving down a Group, there is no significant change in the effective nuclear charge that the electron(s) in the valence shell of the atom experience, as the increasing nuclear charge and increasing shielding effect cancel each other *e.g.*

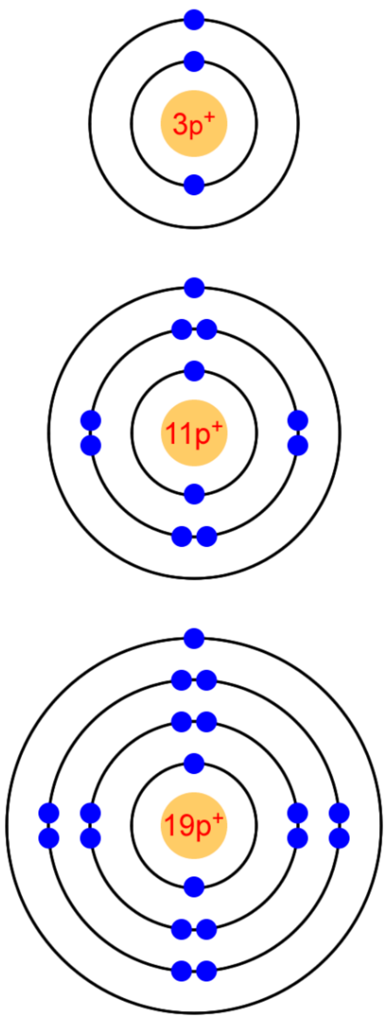
Z_{eff} (Li) = 3 – 2 = +1

Z_{eff} (Na) = 11 – 10 = +1

Z_{eff} (K) = 19 – 18 = +1

Periodic Trends

- First ionization energy *decreases down a Group*.



- The number of protons in the nucleus of an atom (nuclear charge) and the number of electron shells around the nucleus of the atom *both increase* down a Group.

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Periodic Trends

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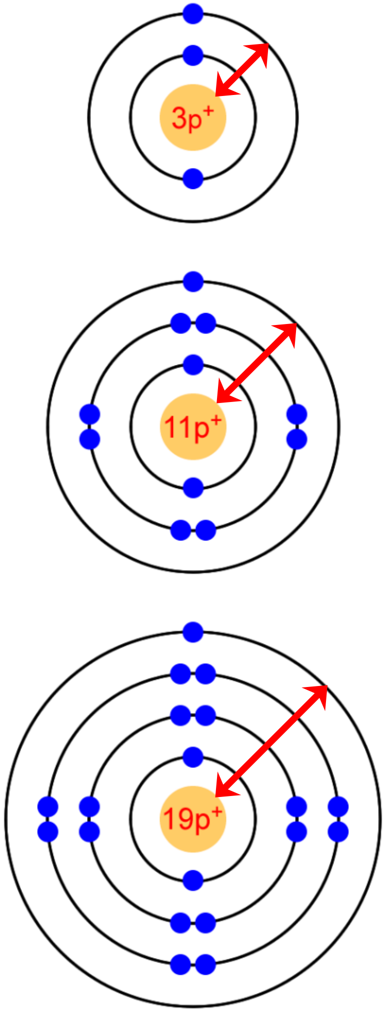


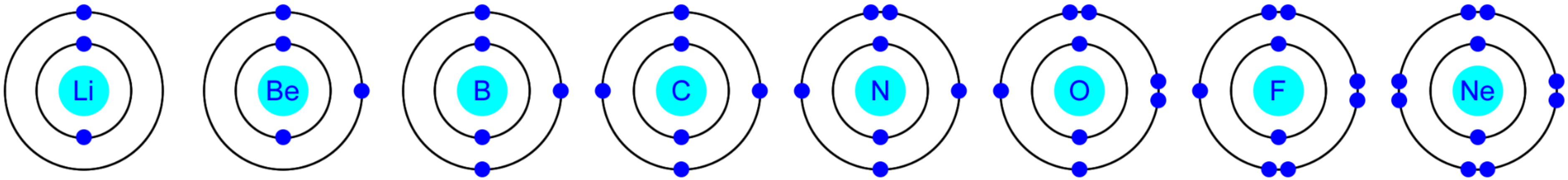
- The addition of a new electron shell to the atoms is significant because it means that the electron(s) in the valence shell (lost during ionization) is *further from the nucleus*.

- This *reduces the electrostatic force of attraction* between the positively charged nucleus and negatively charged electron(s) in the valence shell (inverse square law).

- Less energy is required to remove an electron from the valence shell of the atom, therefore *first ionization energy decreases down a Group*.

Periodic Trends

- First ionization energy *increases across a Period*.



- The number of protons in the nucleus of an atom (nuclear charge) *increases* across a Period.

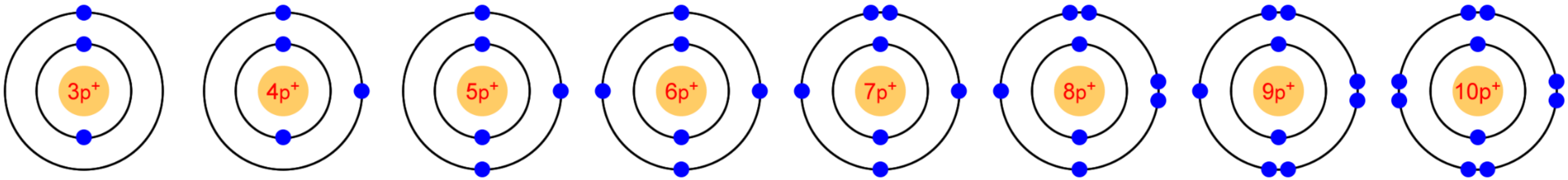
- The number of electron shells *remains constant* across a Period and therefore the number of inner shell electrons available to *shield* electrons in the valence shell from the attractive force of the nucleus *remains constant* across a Period.

- Moving across a Period, electrons in the valence shell of the atom experience a *greater effective nuclear charge*.

Z_{eff} (Li) = 3 – 2 = +1 Z_{eff} (Ne) = 10 – 2 = +8

Periodic Trends

- First ionization energy *increases across a Period*.



- The number of protons in the nucleus of an atom (nuclear charge) *increases* across a Period.

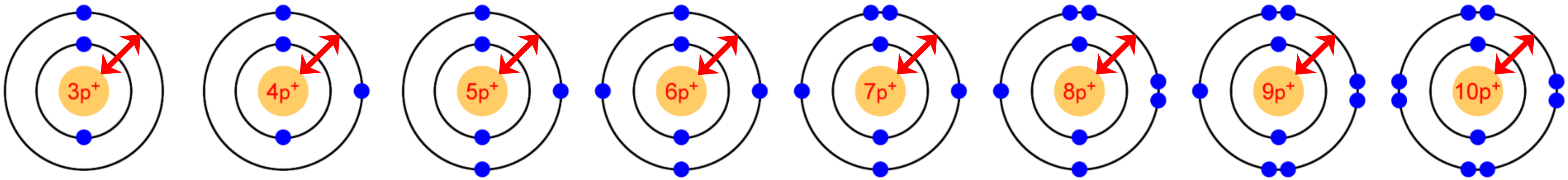
- The number of electron shells *remains constant* across a Period and therefore the number of inner shell electrons available to *shield* electrons in the valence shell from the attractive force of the nucleus *remains constant* across a Period.

- Moving across a Period, electrons in the valence shell of the atom experience a *greater effective nuclear charge*.

Z_{eff} (Li) = 3 – 2 = +1 Z_{eff} (Ne) = 10 – 2 = +8

Periodic Trends

- First ionization energy *increases across a Period*.

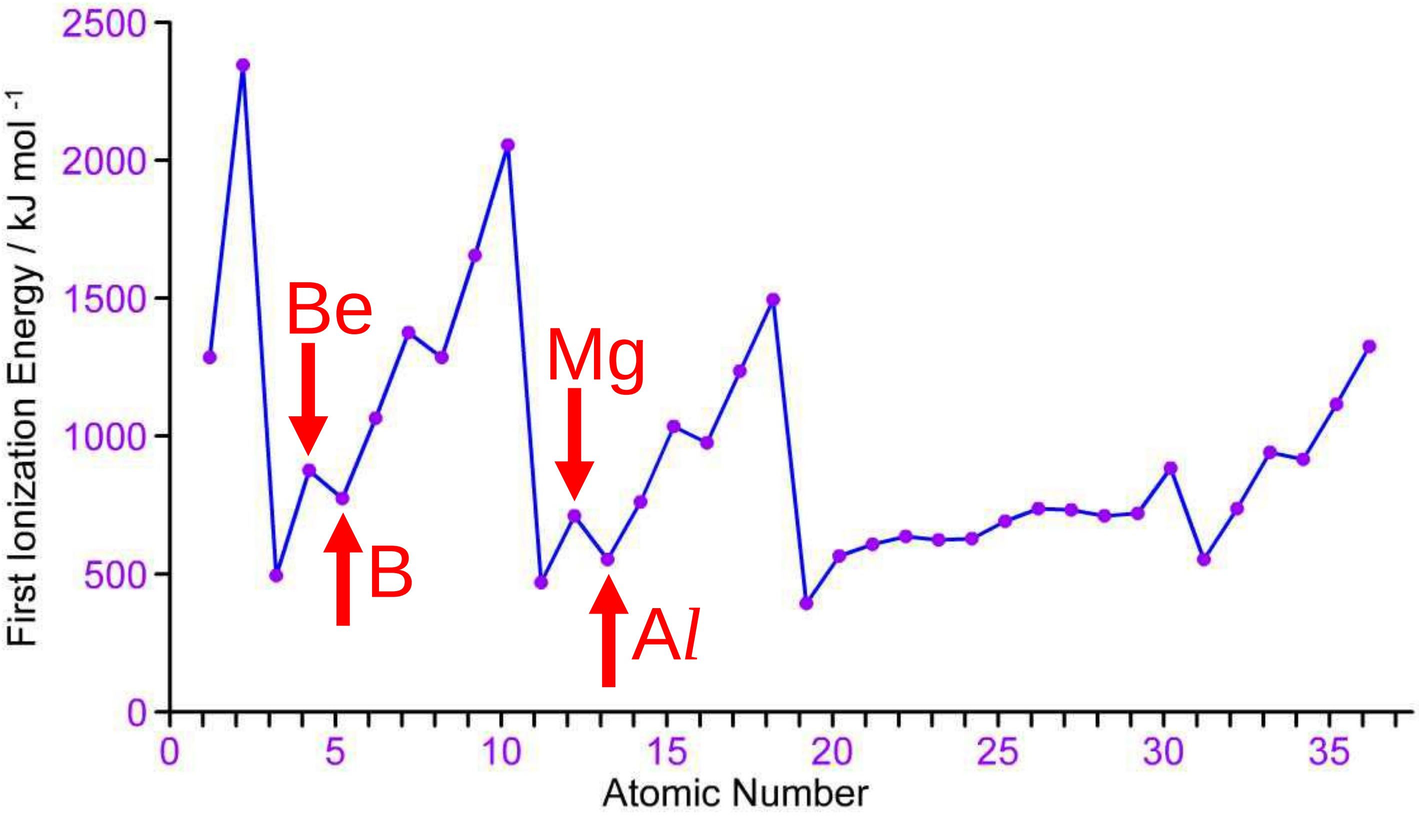


- An increase in effective nuclear charge means that there is an *increase in the electrostatic force of attraction* between the positively charged protons in the nucleus and negatively charged electron(s) in the valence shell of the atom – which are the electrons that are lost during ionization.

- Moving across a Period, more energy is required to remove an electron from the valence shell of an atom, hence *first ionization energy increases across a Period*.

Periodic Trends

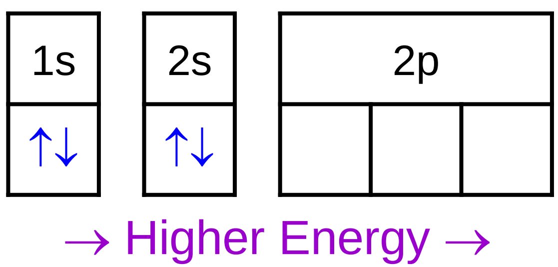
- First ionization energy *decreases* slightly between *Group 2 and Group 13* elements.



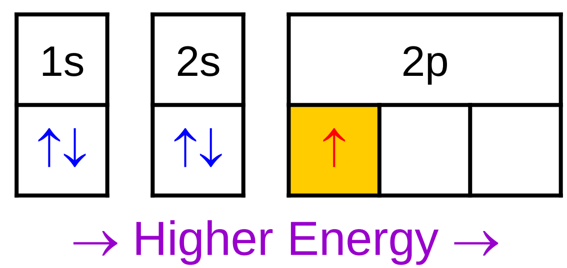
Periodic Trends

- First ionization energy *decreases* slightly between *Group 2 and Group 13* elements.
- Moving from Group 2 to Group 13, the additional electron enters a *p*-orbital of the same principle quantum shell.
- An electron in a *p*-orbital is *higher in energy* than an electron in the *s*-orbital of the same principle quantum shell. Consequently, *less energy* is required to remove the *p*-orbital electron (ionization) compared to an electron in the corresponding *s*-orbital, and first ionization energy *decreases* slightly between Group 2 and Group 13.

Beryllium
Group 2

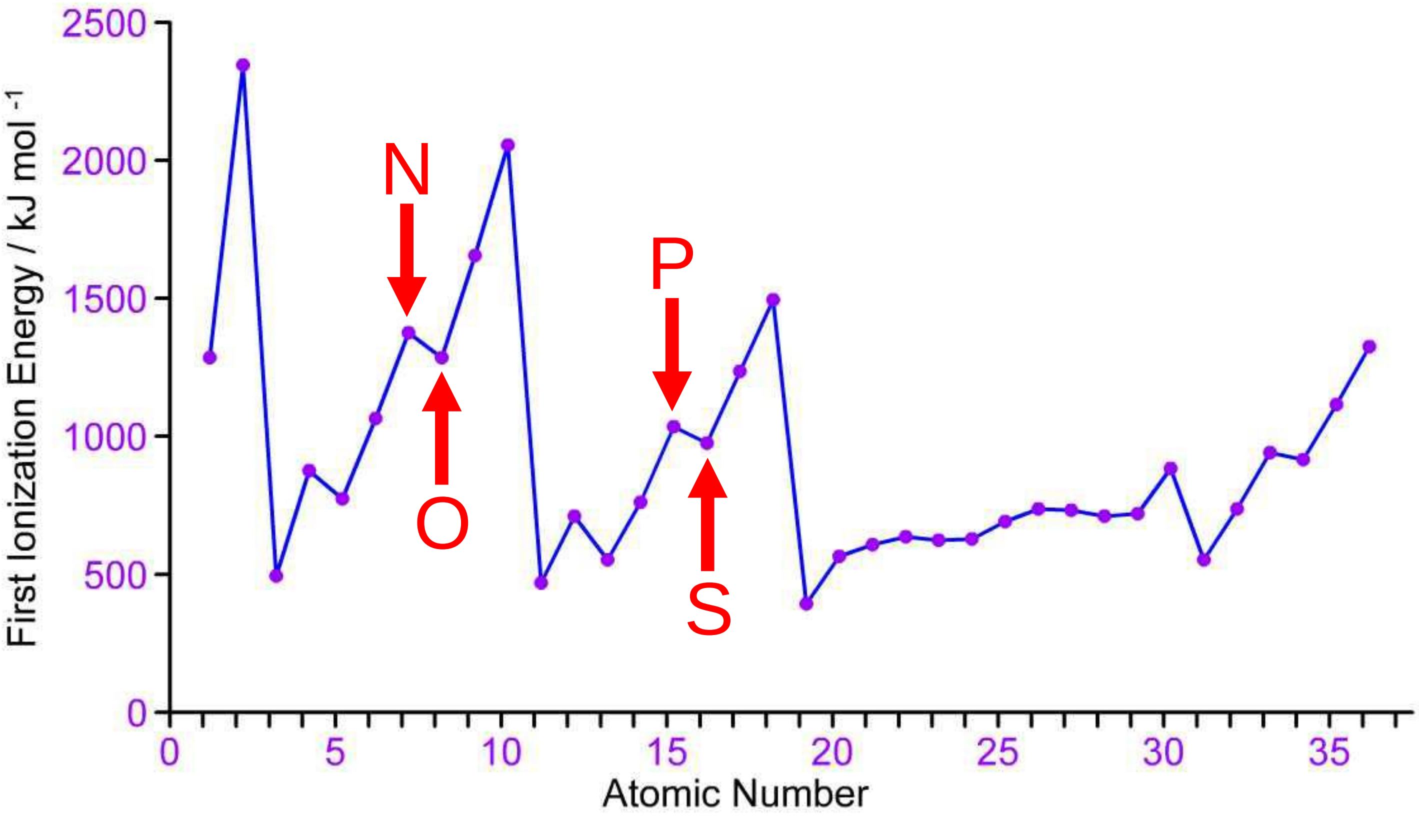


Boron
Group 3



Periodic Trends

- First ionization energy *decreases* slightly between *Group 15* and *Group 16* elements.



Periodic Trends

- First ionization energy *decreases* slightly between *Group 15* and *Group 16* elements.

- Moving from Group 15 to Group 16, the additional electron must spin pair with an existing electron in one of the atom’s *p*-orbitals.

- An *electrostatic force of repulsion* between the two spin paired electrons that share the same *p*-orbital means that *less energy* is required to remove (ionization) an electron from the *p*-orbital, and first ionization energy *decreases* slightly between Group 15 and Group 16.

Nitrogen
Group 15

1s	2s	2p		
↑↓	↑↓	↑	↑	↑

→ Higher Energy →

Oxygen
Group 16

1s	2s	2p		
↑↓	↑↓	↑↓	↑	↑

→ Higher Energy →

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End of Presentation

Advanced Theories of Atomic Structure

Presentation on
Advanced Theories of Atomic Structure
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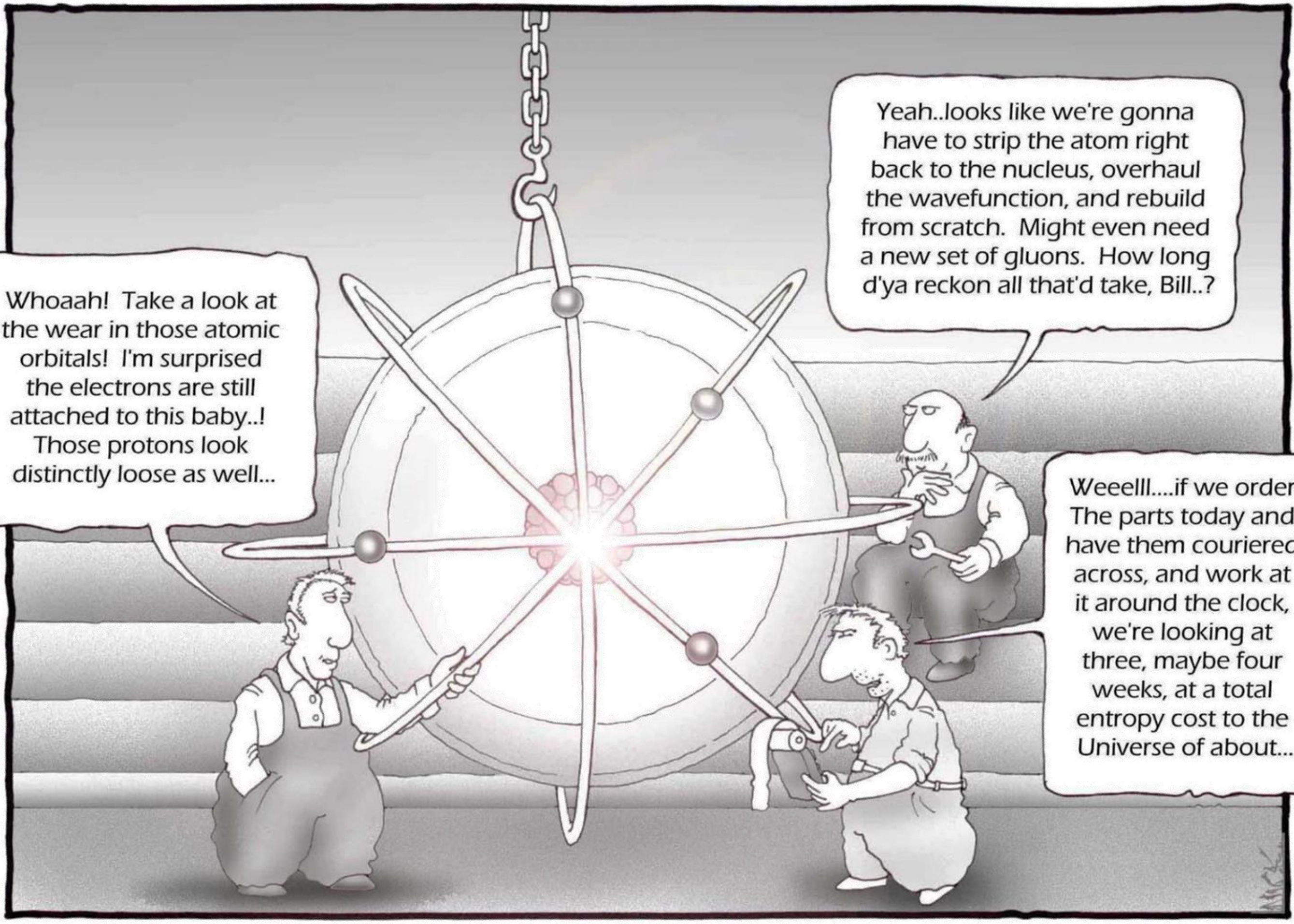
8th January 2017

Advanced Theories of Atomic Structure



Quantum mechanics.