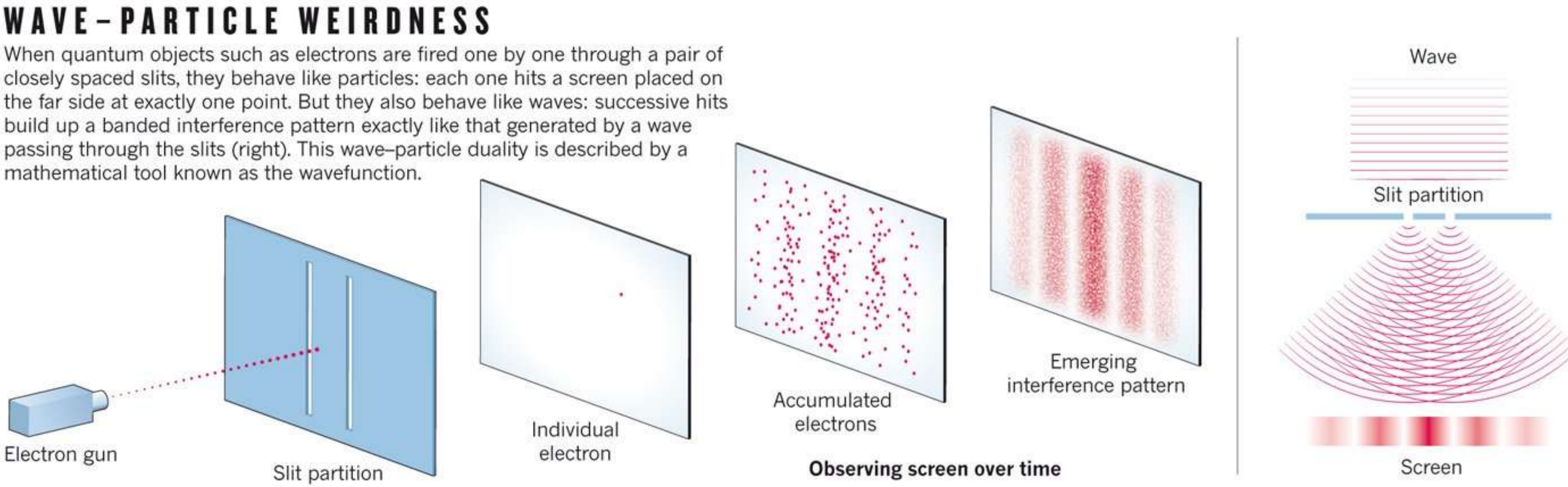
WAVE QUANTUM MECHANIC MODEL

WAVE QUANTUM MECHANIC THEORY

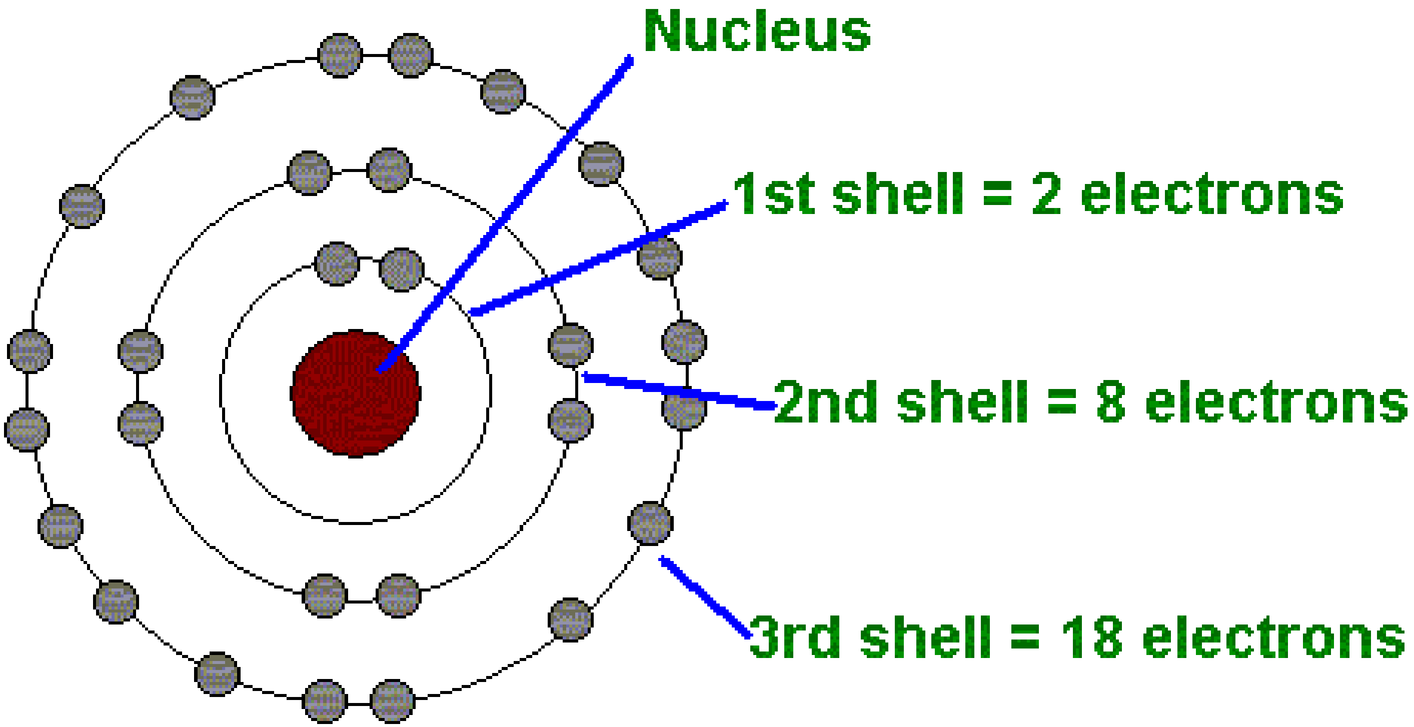
WAVE QUANTUM MECHANIC THEORY

quantum mechanics – mathematical description of **wave-particle duality** of energy / matter



PREVIOUS ATOMIC MODEL

Old model:



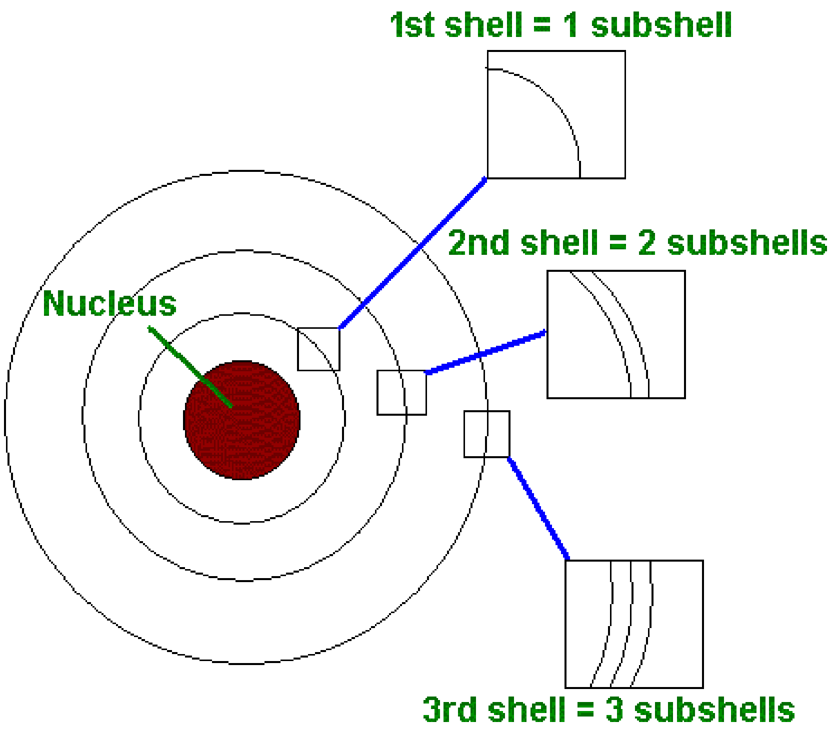
Electrons occupy specific energy levels/shells in an atom.

number of electrons per level = $2n^2$

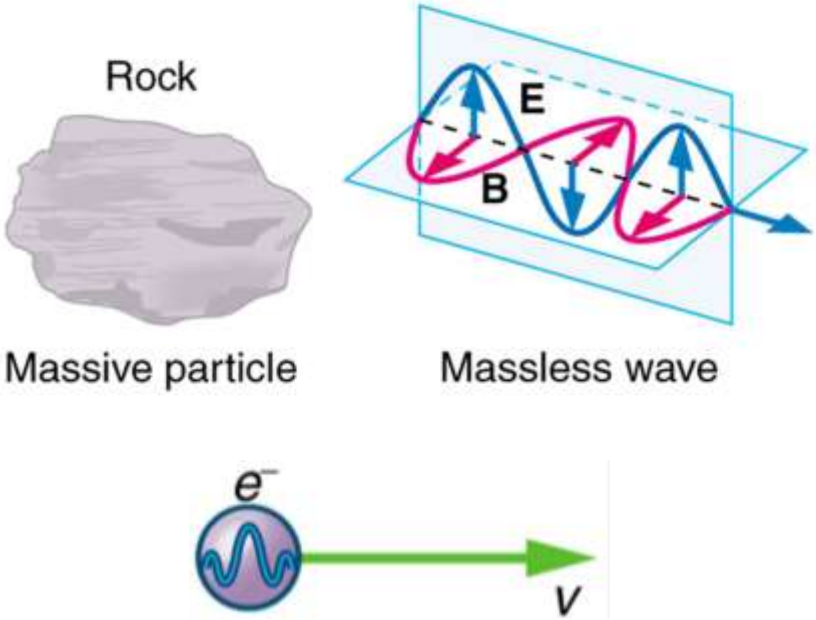
SCHRÖDINGER

Erwin Schrödinger proposed that:

1) Each energy level had sub-levels



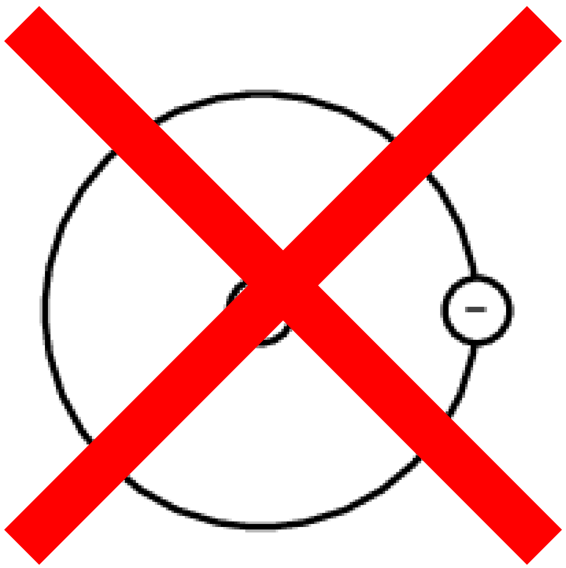
2) Electrons are both particles and waves at the same time (not localized in 2-D orbits)



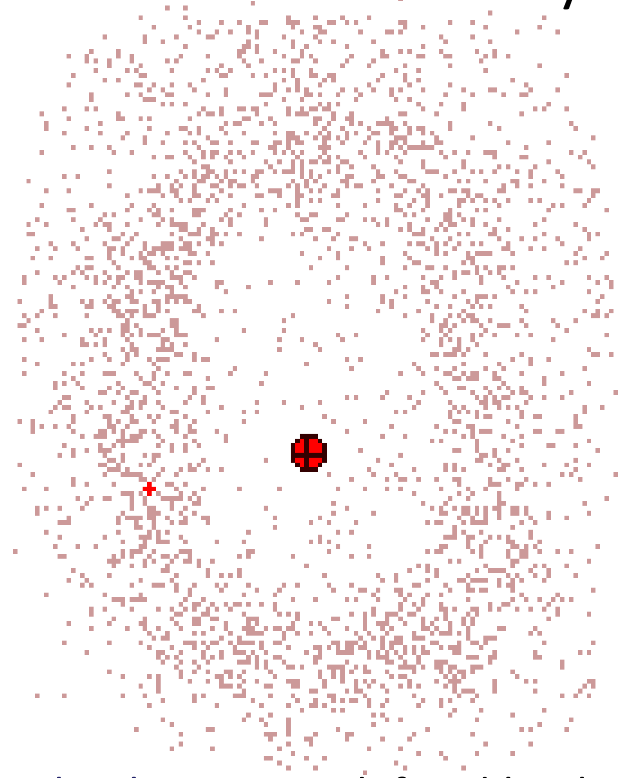
HEISENBERG UNCERTAINTY PRINCIPLE

Heisenberg's Uncertainty Principle

- cannot predict speed and location at the same time for very small particles



vs.



orbit – a defined 2-D circle/ellipse around a nucleus where an e^- is found

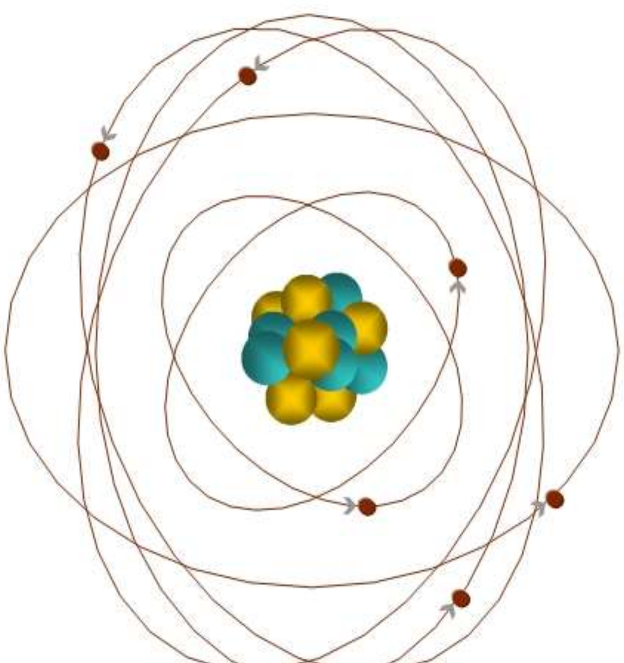
orbital – a space defined by the Schrödinger Wave Equation around a nucleus where an e^- is *probably* found

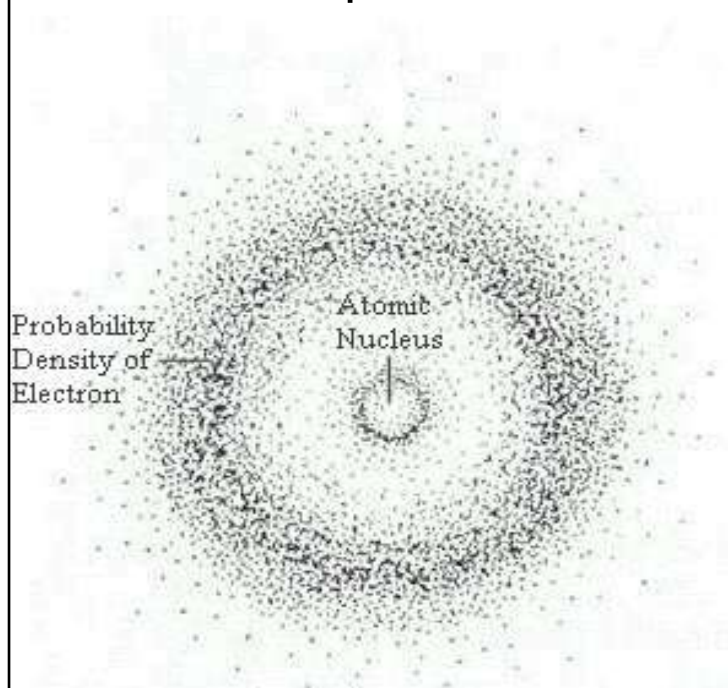
$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \hat{H}\Psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\Psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t)$$

ORBITS VS ORBITALS

Orbits Vs. Orbitals

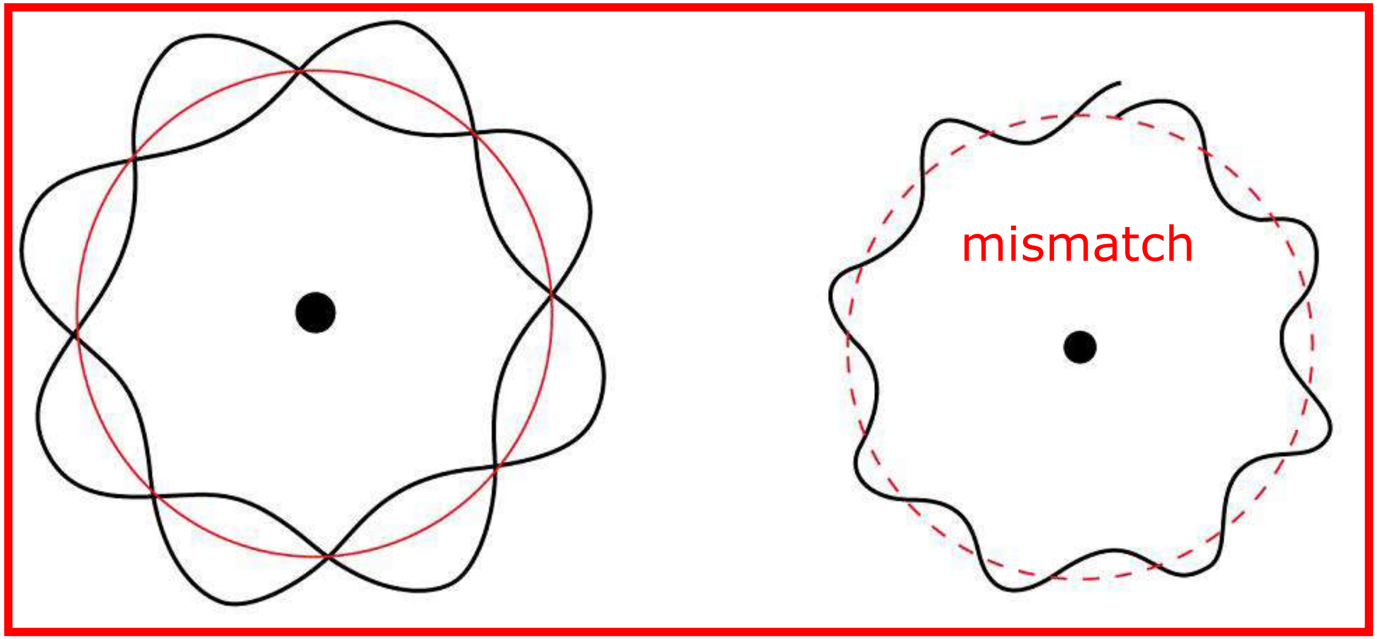
2-D path	3-D path
Fixed distance from nucleus	Variable distance from nucleus
Circular or elliptical path	No path; varied shape of region
$2n^2$ electrons per orbit	2 electrons per orbital





FIXED ENERGY LEVELS ONLY

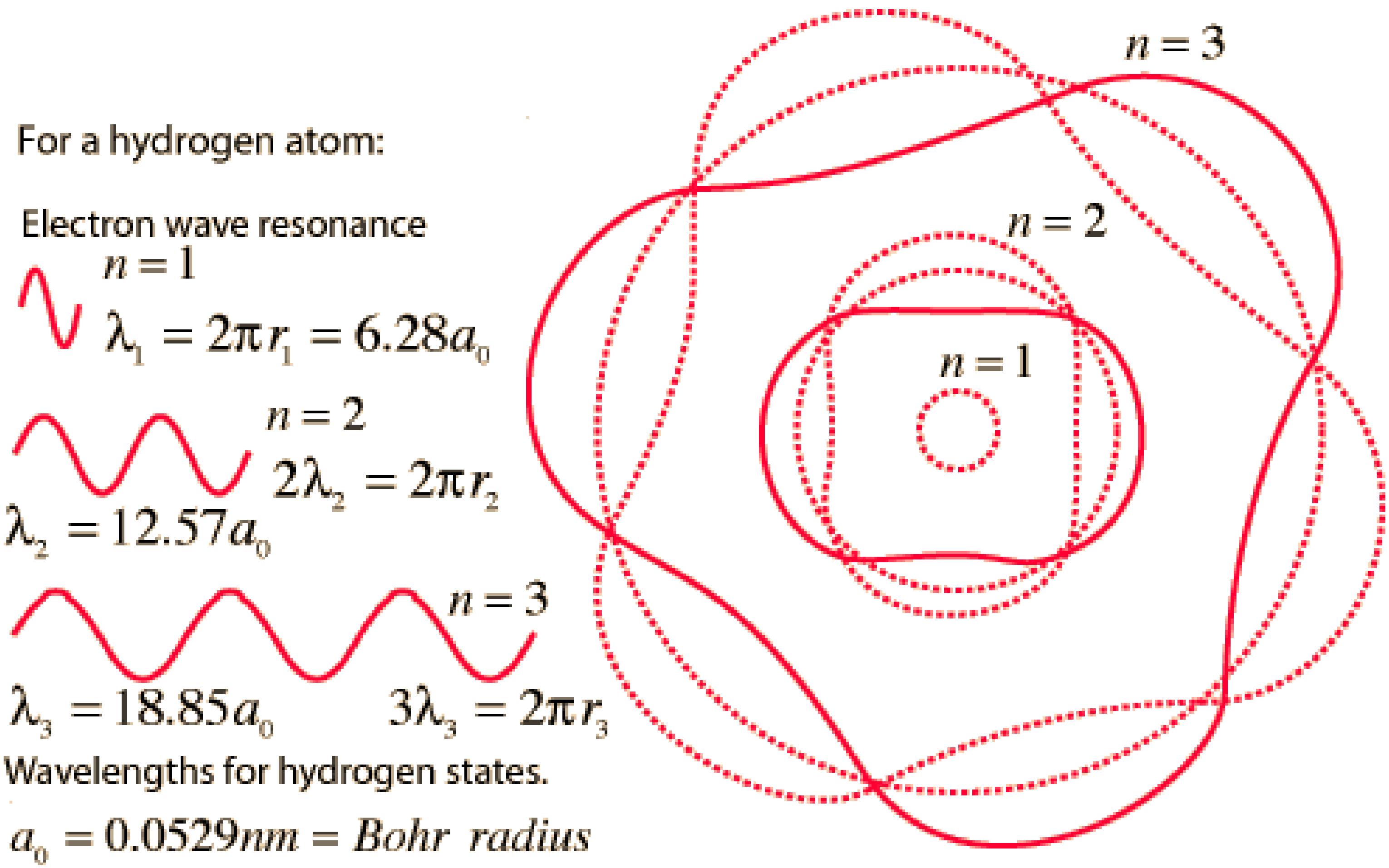
Since electrons are like waves around the nucleus, they cannot have wavelengths that result in destructive interference (which can collapse the wave).



As a result, the wavelengths must be multiples of whole numbers (n = 1, 2, 3, 4, …), which explains why there are areas where electrons cannot exist.

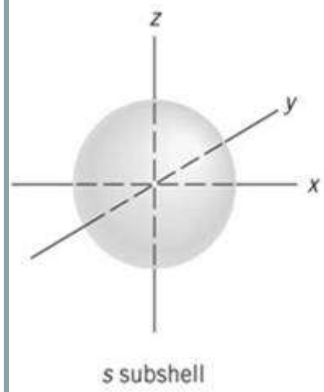
FIXED ENERGY LEVELS ONLY

This causes electrons to be confined to certain probabilities (orbitals) around the nucleus.

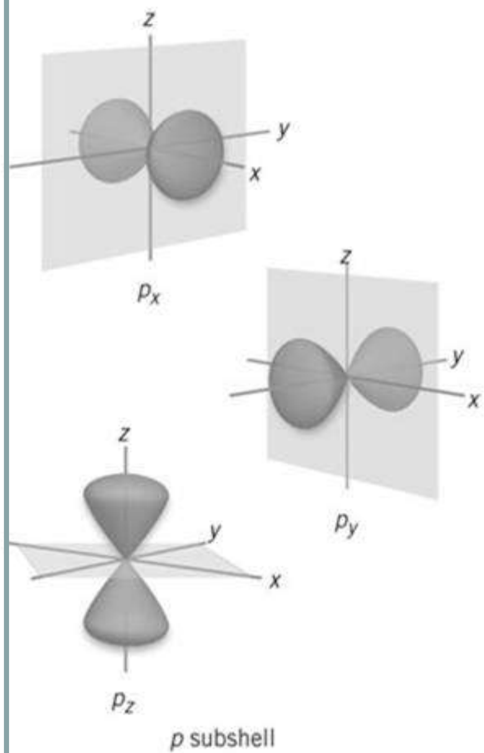


ORBITAL SHAPES

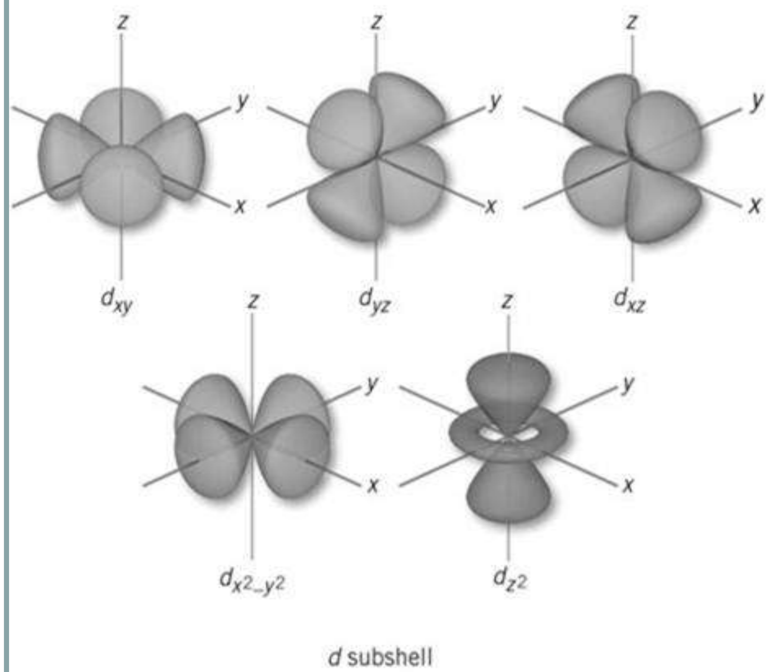
Each orbital (containing 2 electrons) is further classified under different categorizations based on their shape



s - orbital



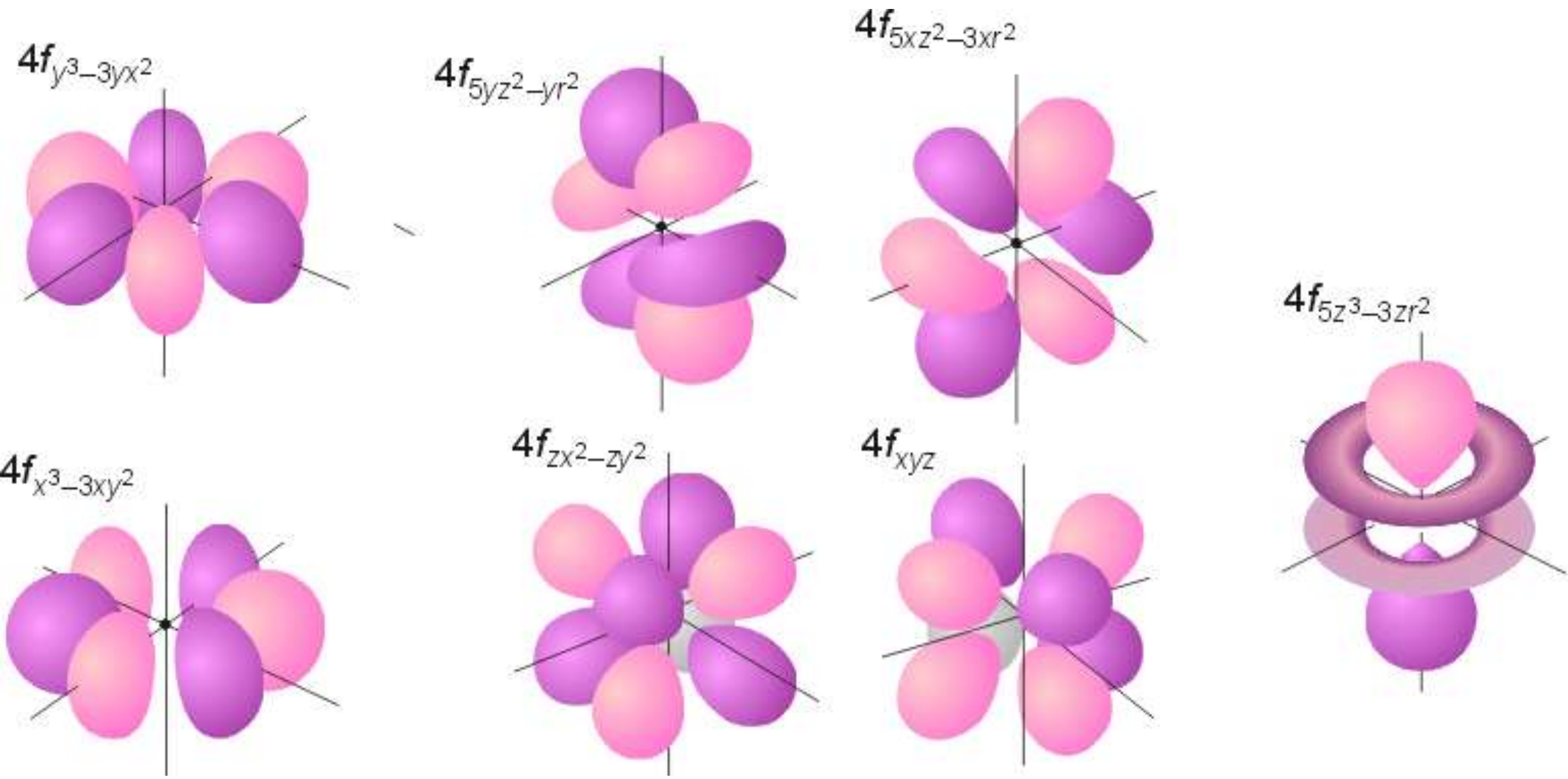
p - orbitals



d - orbitals

ORBITAL SHAPES

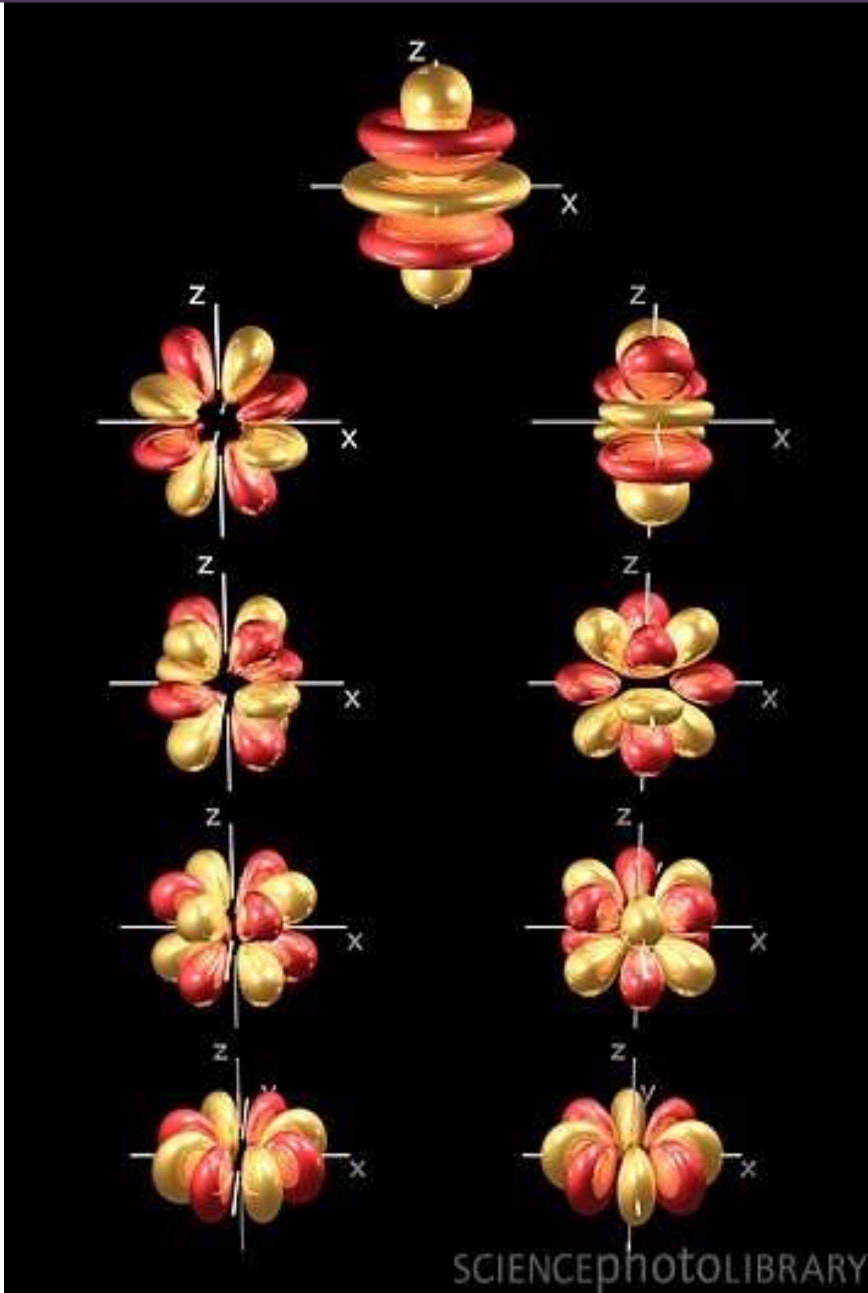
f- orbitals



ORBITAL SHAPES

g – orbitals

Orbital shapes are energy dependent and can be solved through Schrödinger's wave equation.

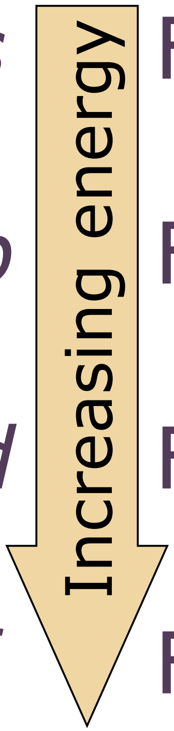


ORBITAL SHAPES

Summary of s, p, d, f orbitals:

Value of l	Sublevel Symbol	Number of Orbitals
0	s (sharp)	1
1	p (principle)	3
2	d (diffuse)	5
3	f (fundamental)	7

ORBITAL CAPACITY

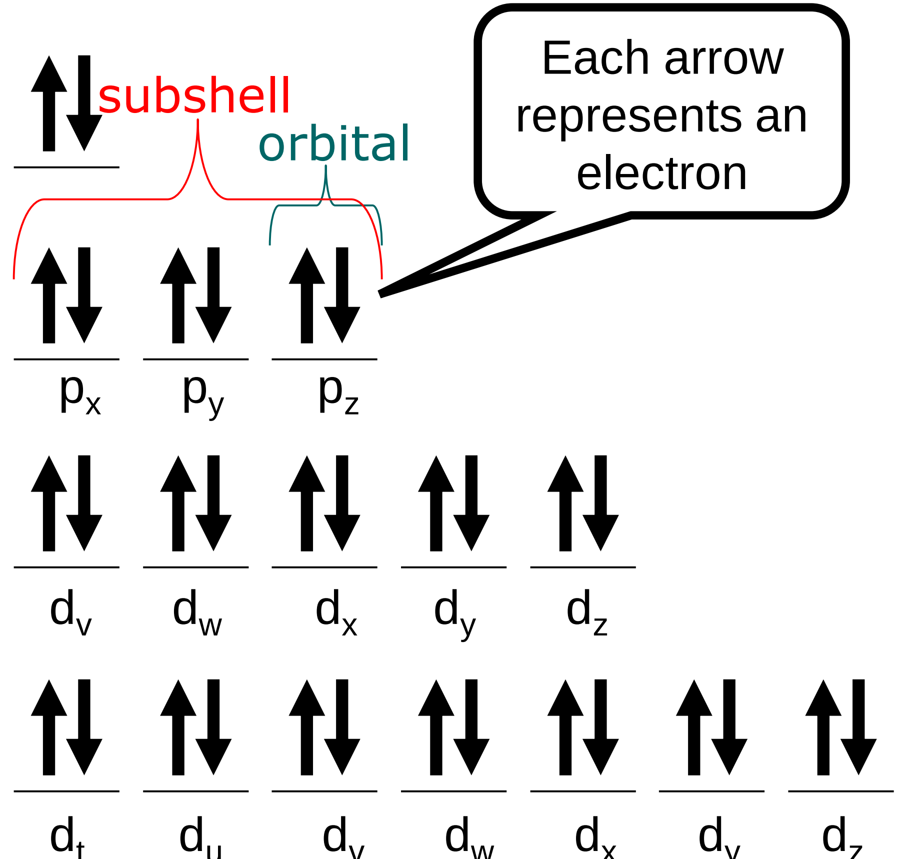


s Fits 2 electrons

p Fits 6 electrons

d Fits 10 electrons

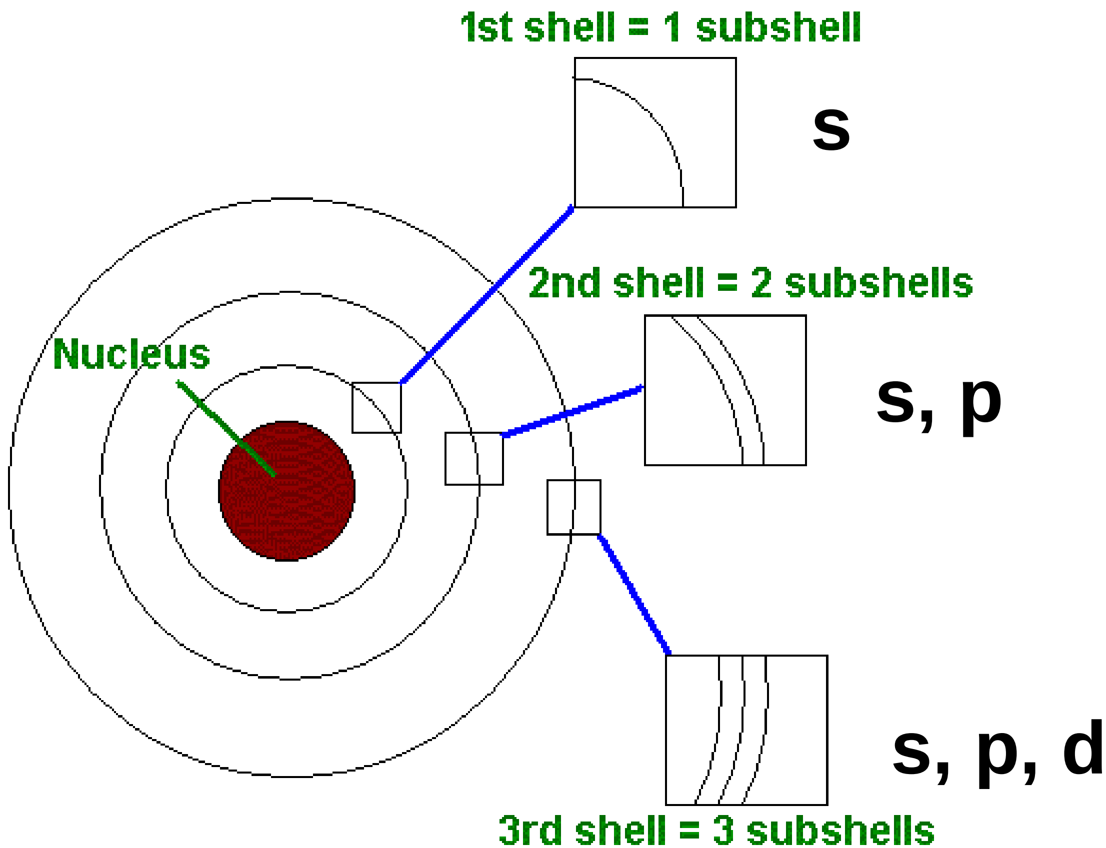
f Fits 14 electrons



Pauli exclusion principle: No two electrons in an orbital have the same direction (all electrons have angular momentum causing it to have a magnetic direction)

SUBSHELLS IN EACH SHELL

RECALL: Schrödinger proposed that each energy level/shell had a respective number of subshells.



What do you think these subshells are?

SUMMARY

Electron distribution:

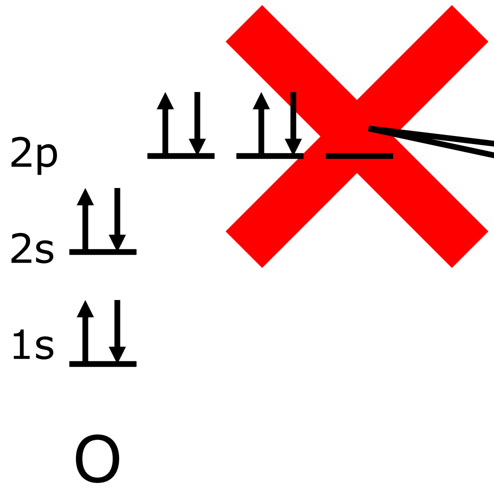
Energy Level	Sublevel	Maximum # of Electrons in Energy Level ($2n^2$)	Number of Each Orbital	Maximum # of Electrons in Orbital Type
1	s	2	1	2
2	s p	8	1 3	2 6
3	s p d	18	1 3 5	2 6 10
4	s p d f	32	1 3 5 7	2 6 10 14

ELECTRON ENERGY-LEVEL DIAGRAMS

Drawing an **electron energy-level diagram**

Example: Oxygen

How many electrons does oxygen have? **8**



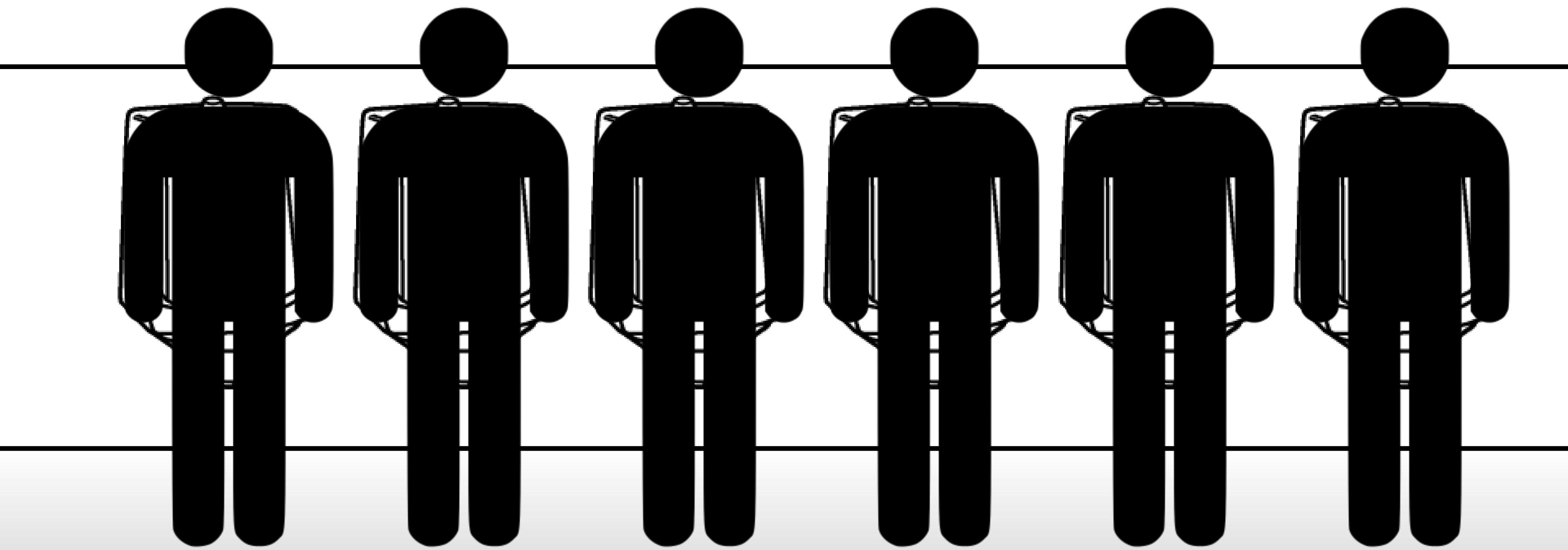
Hund's rule: No two electrons can be put into the same orbital until one electron has been put into each of the equal-energy orbitals

aufbau principle: An energy sublevel must be filled before moving to the next higher sublevel

ELECTRON ENERGY-LEVEL DIAGRAMS

Drawing an **electron energy-level diagram**

Hund's rule analogy:



ELECTRON ENERGY-LEVEL DIAGRAMS

Drawing an **electron energy-level diagram**

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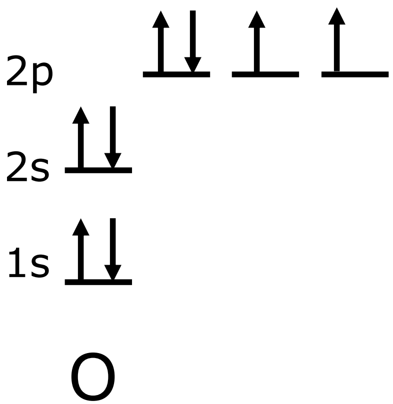

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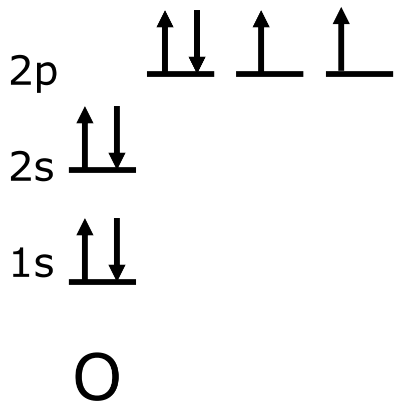
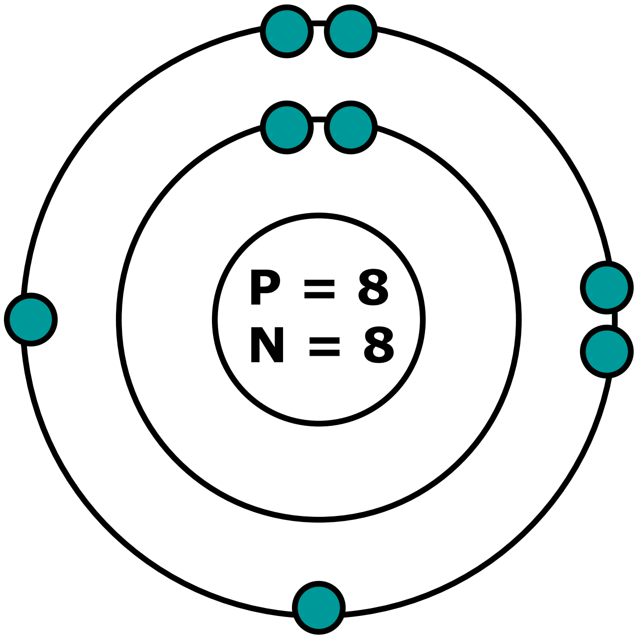
ELECTRON ENERGY-LEVEL DIAGRAMS

Drawing an **electron energy-level diagram**

Example: Oxygen



Compare with its Bohr-Rutherford diagram:



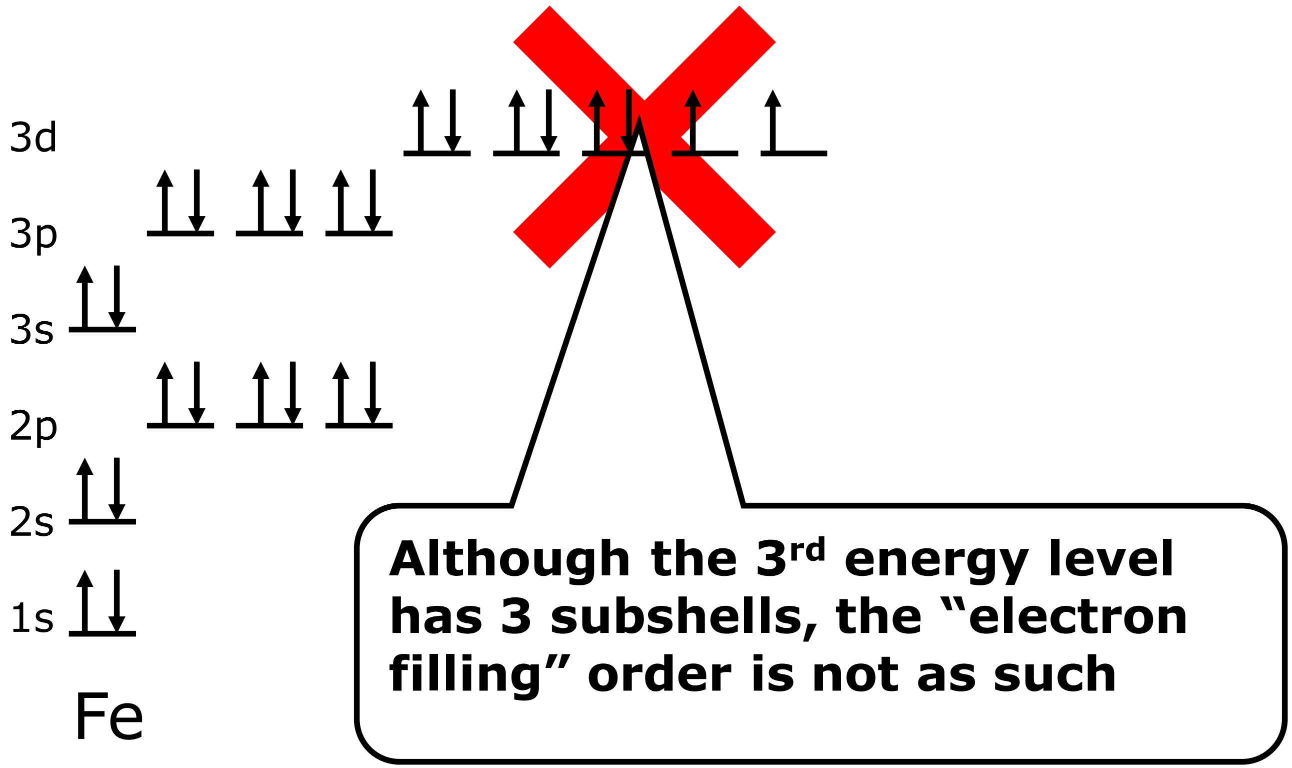
Notice how the pairing of electrons in the Bohr-Rutherford diagram matches the energy level diagram

ELECTRON ENERGY-LEVEL DIAGRAMS

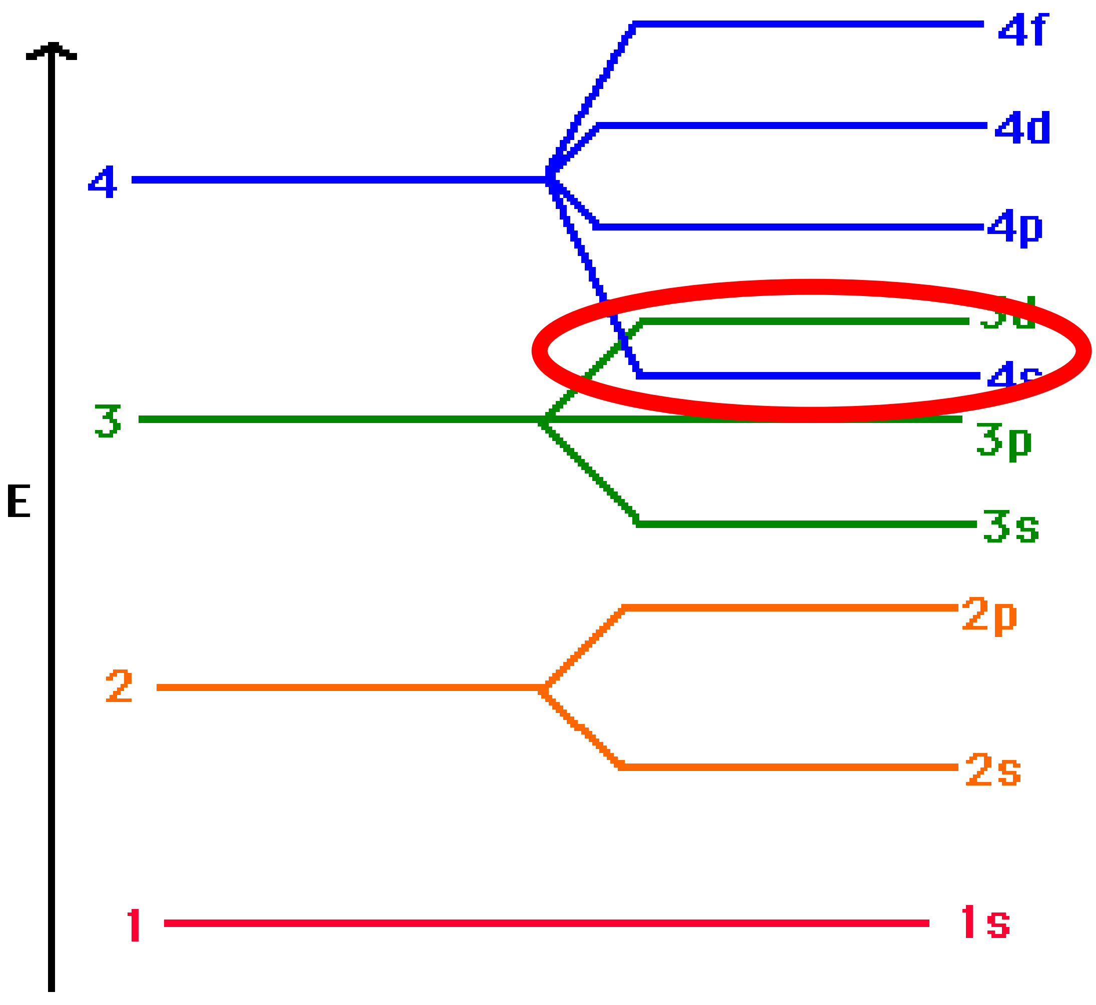
Drawing an **electron energy-level diagram**

Example: Iron

How many electrons does iron have? **26**



ELECTRON ENERGY-LEVEL DIAGRAMS



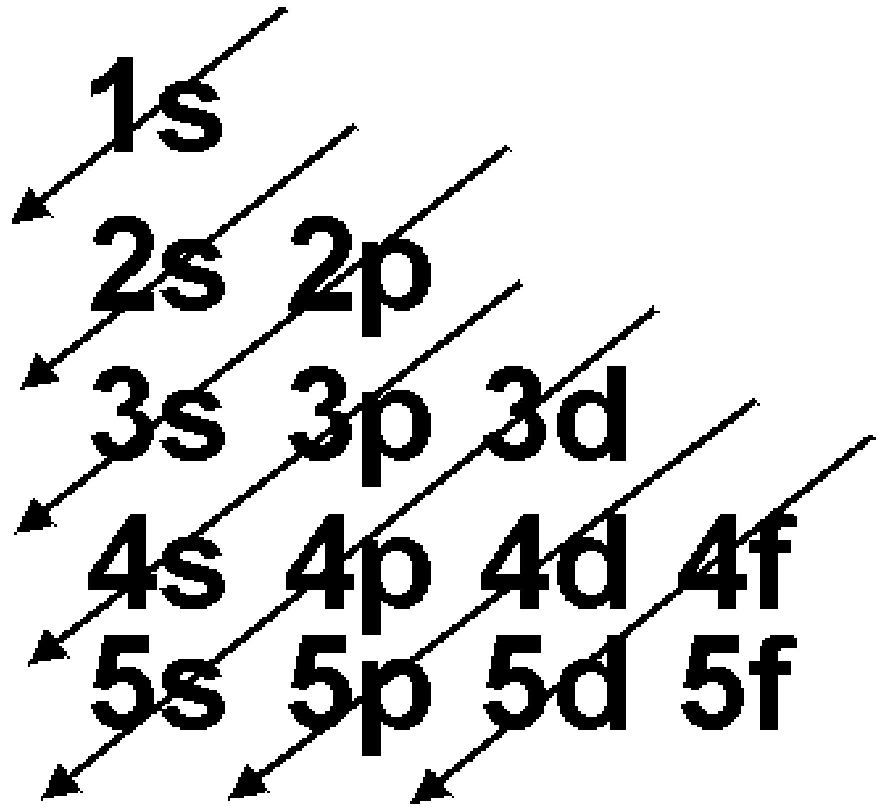
Each energy level is supposed to begin with one s orbital, and then three p orbitals, and so forth.

There is often a bit of overlap.

In this case, the 4s orbital comes before the 3d orbitals.

ELECTRON ENERGY-LEVEL DIAGRAMS

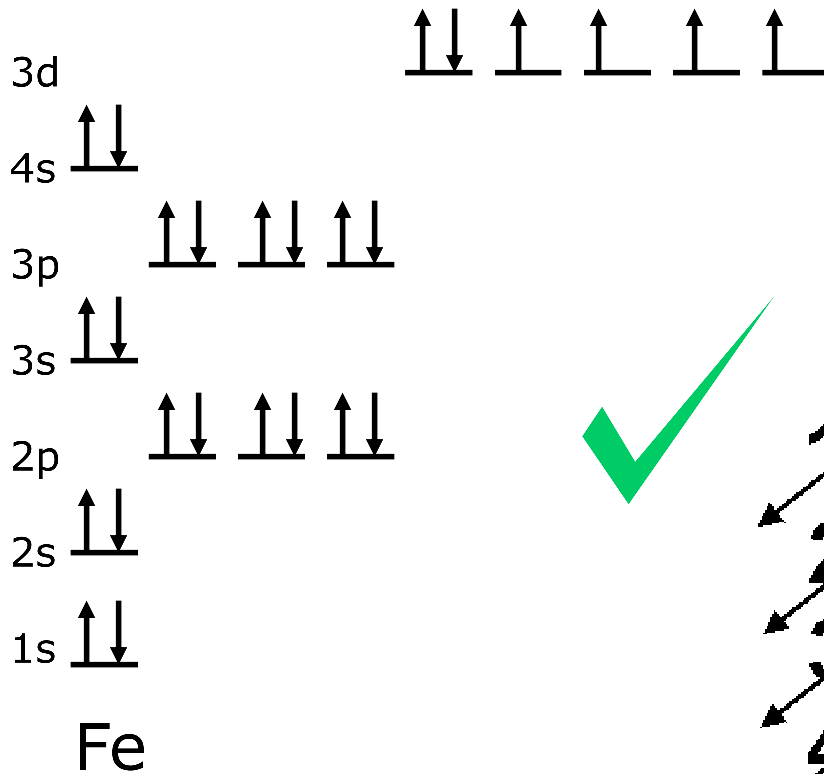
aufbau diagram: Start at the top and add electrons in the order shown by the diagonal arrows.

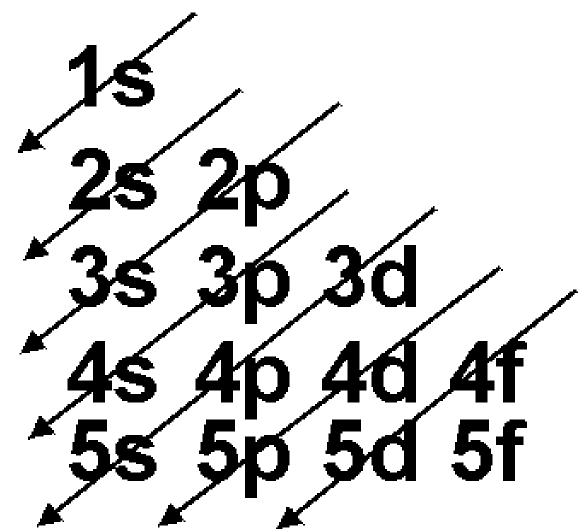


ELECTRON ENERGY-LEVEL DIAGRAMS

Drawing an **electron energy-level diagram**

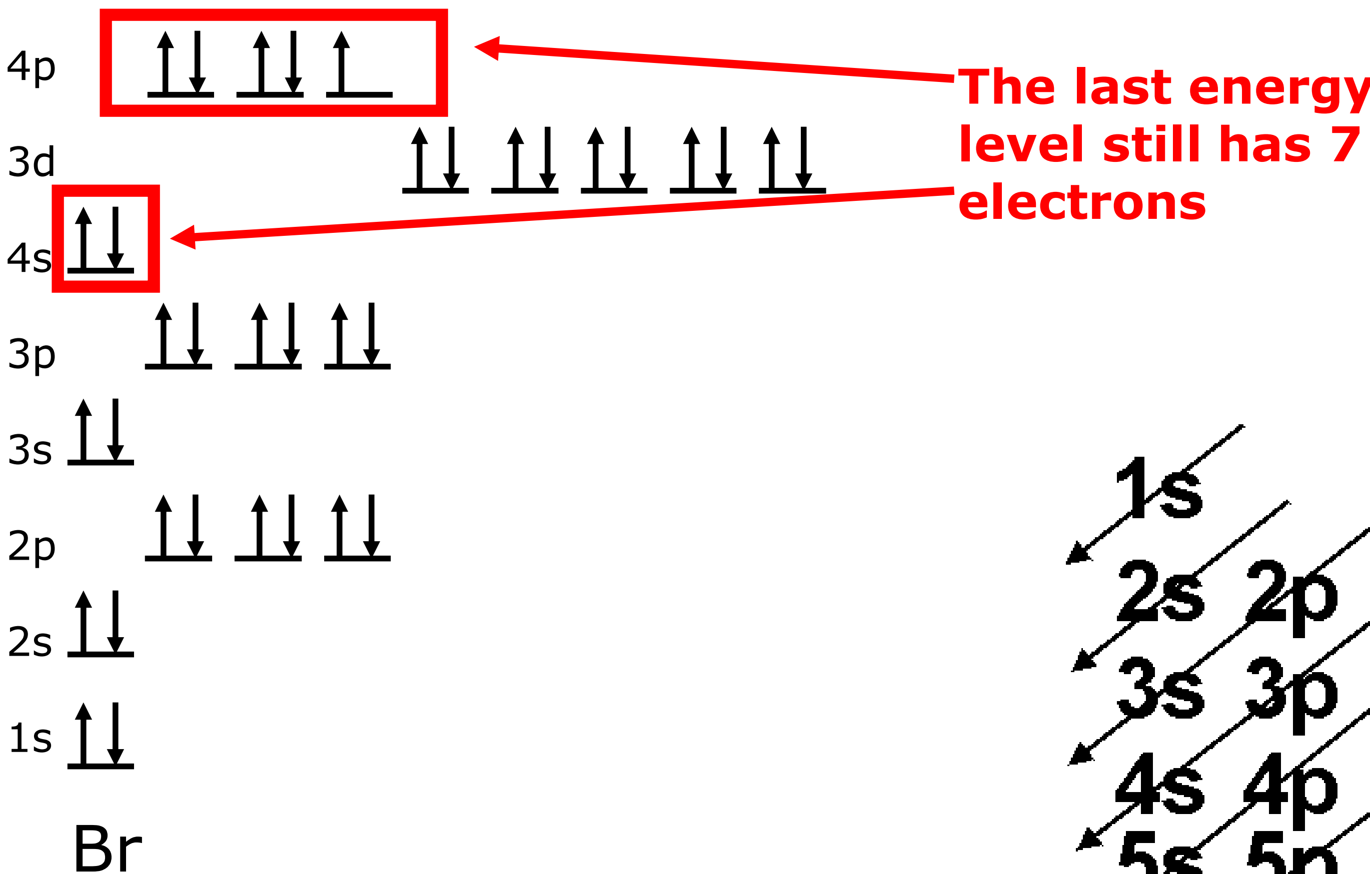
Example: Iron   How many electrons does iron have? **26**

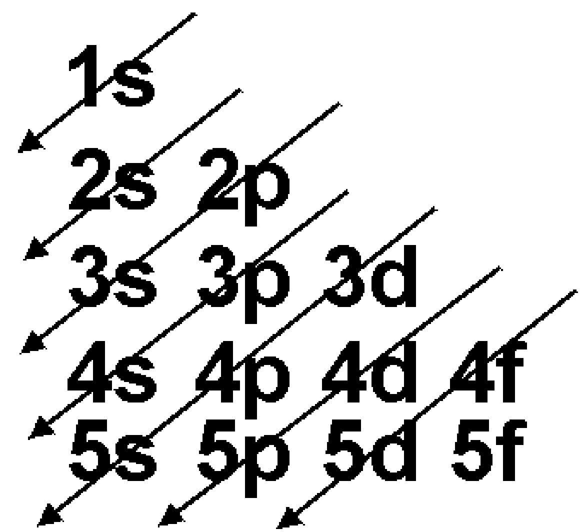




ELECTRON ENERGY-LEVEL DIAGRAMS

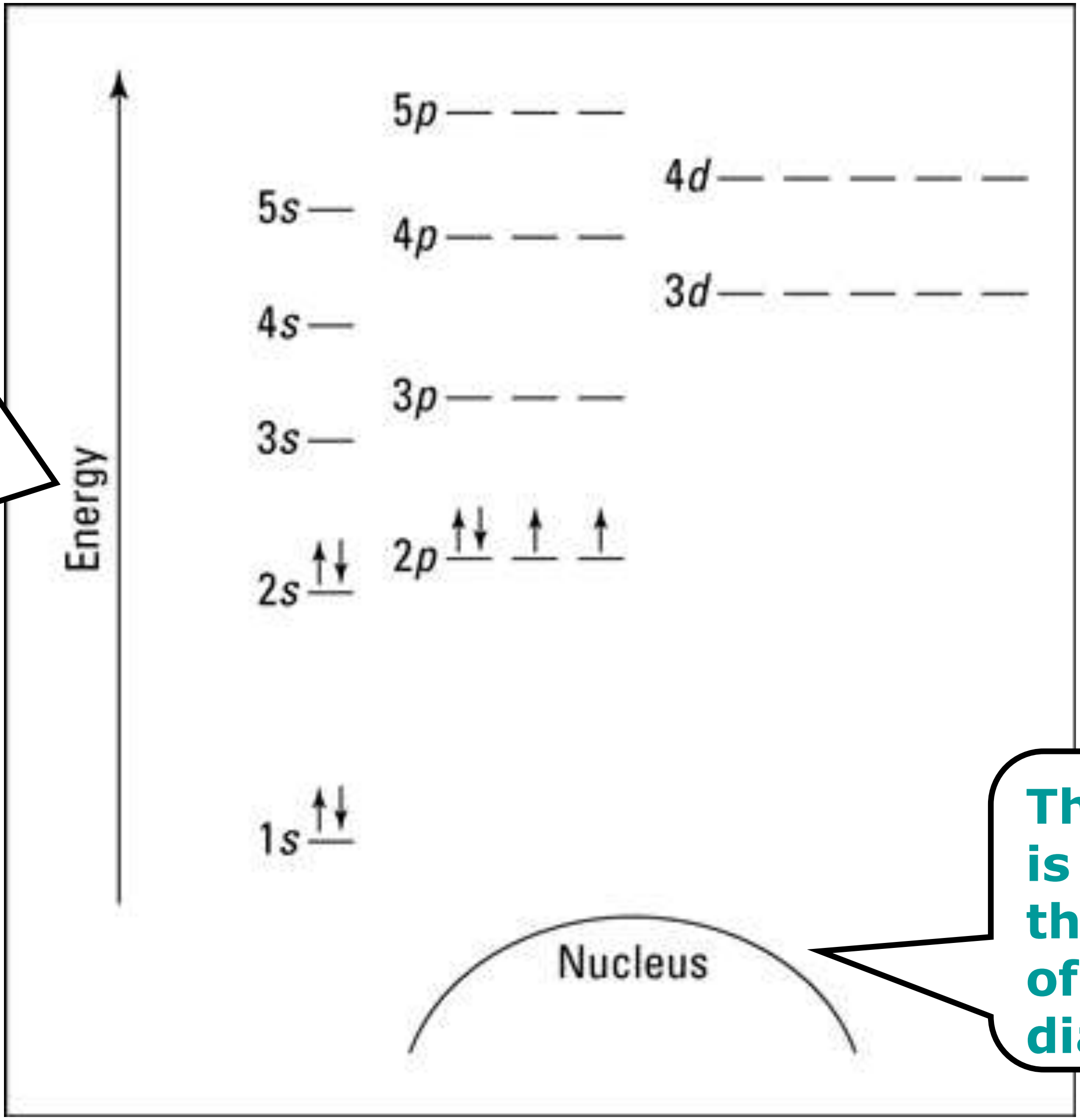
So why does bromine still have 7 valence electrons despite how the 3rd energy level can hold 18 electrons?





ELECTRON ENERGY-LEVEL DIAGRAMS

Why is an electron energy-level diagram drawn as such?



The greater the orbital number, the greater the energy of the electrons

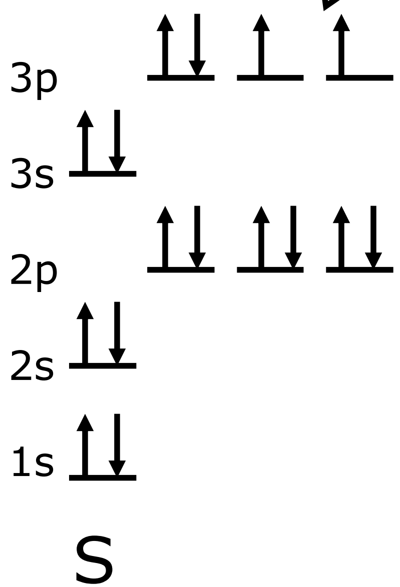
The nucleus is located at the bottom of the diagram

IONS

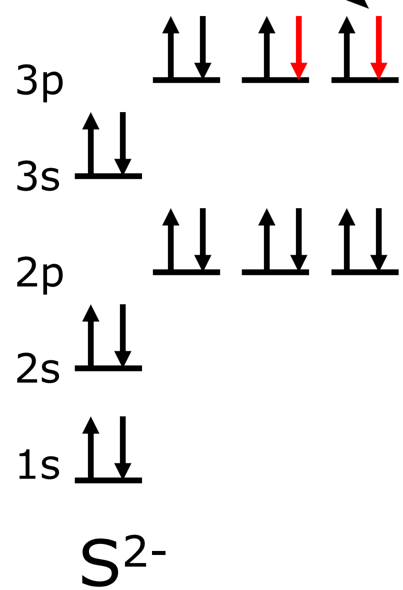
Drawing an **electron energy-level diagram**

Example: sulfur vs sulfide ion

Observe how there are two unpaired electrons in sulfur



This explains why sulfur gains 2 electrons in ionic form



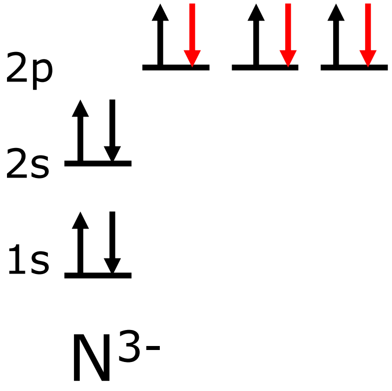
*This is despite the fact that sulfur has 5 unfilled **d** orbitals*

IONS

General rule for anions:

Add the extra electrons corresponding to the ion charge to the total number of electrons

Example: N^{3-}

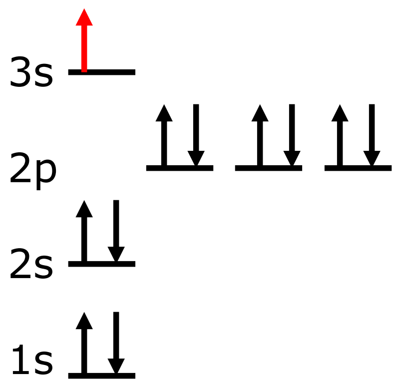


IONS

General rule for cations:

Remove the number of electrons corresponding to the charge from the orbitals within the highest energy level number

Example: Na^+

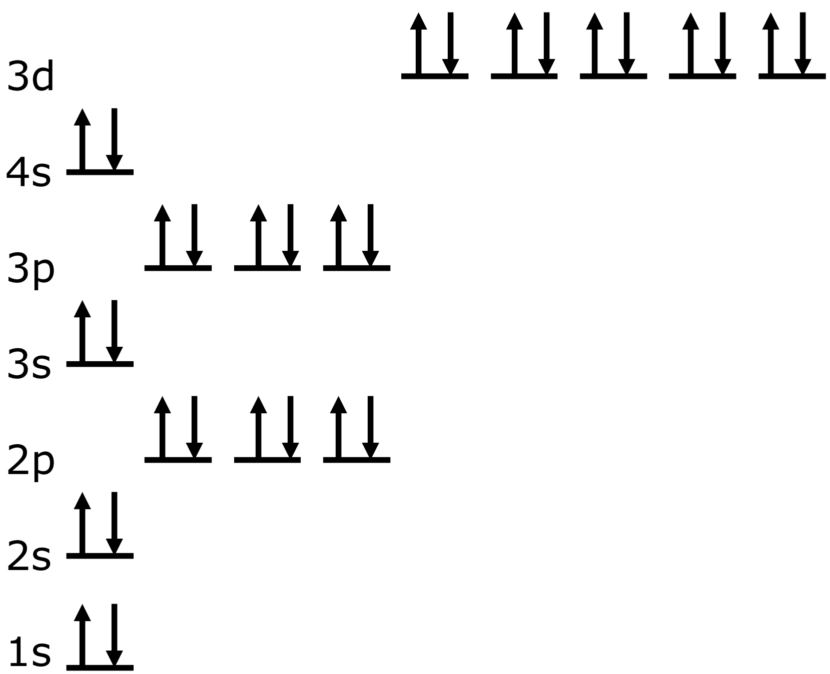


Na^+

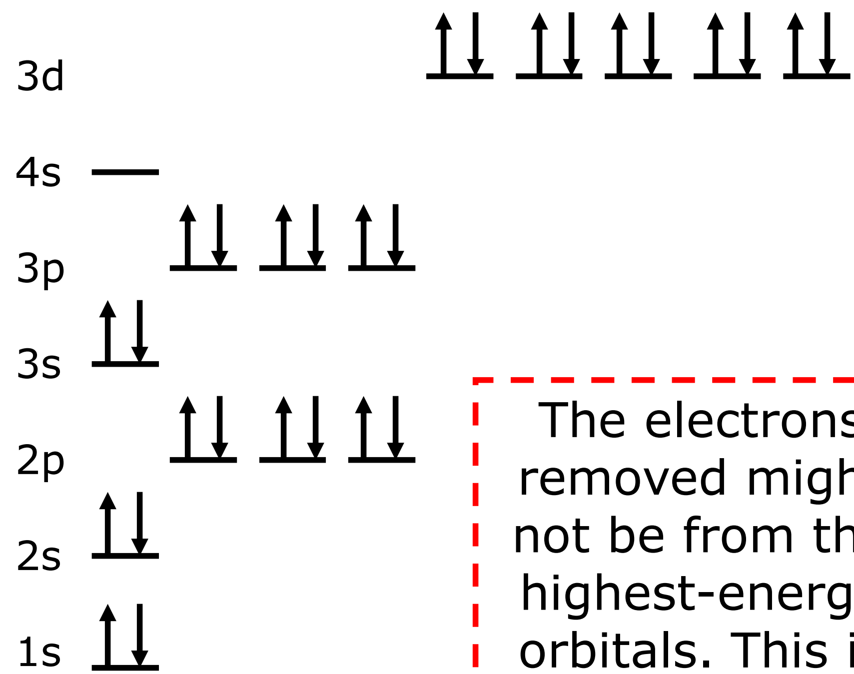
EXCEPTIONS TO AUFBAU PRINCIPLE

Exception to Aufbau Principle:

Example: zinc vs zinc ion



Zn



Zn^{2+}

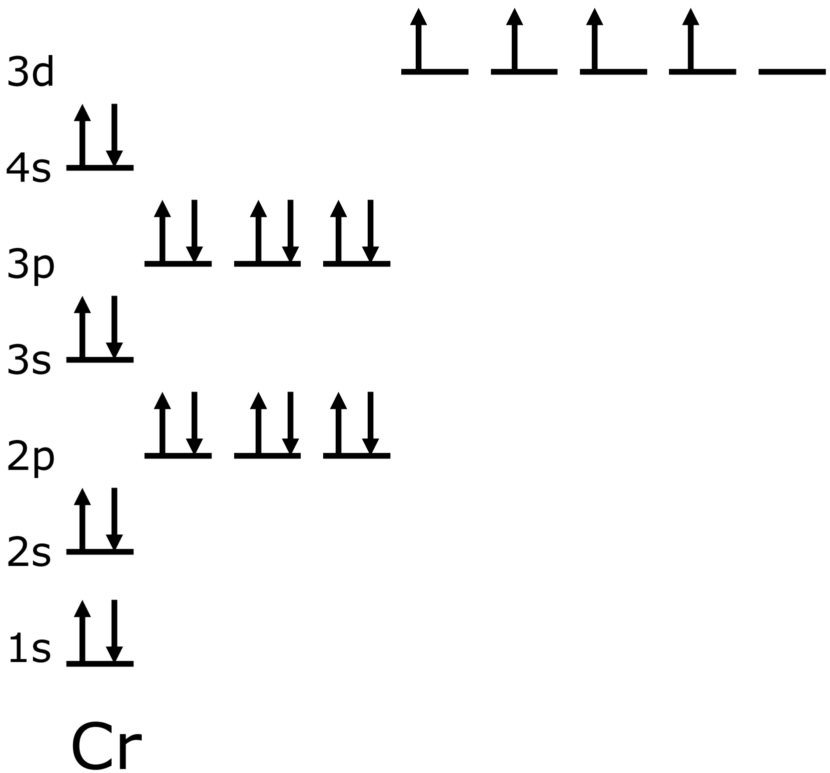
The electrons removed might not be from the highest-energy orbitals. This is based on experimental evidence.

EXCEPTIONS TO AUFBAU PRINCIPLE

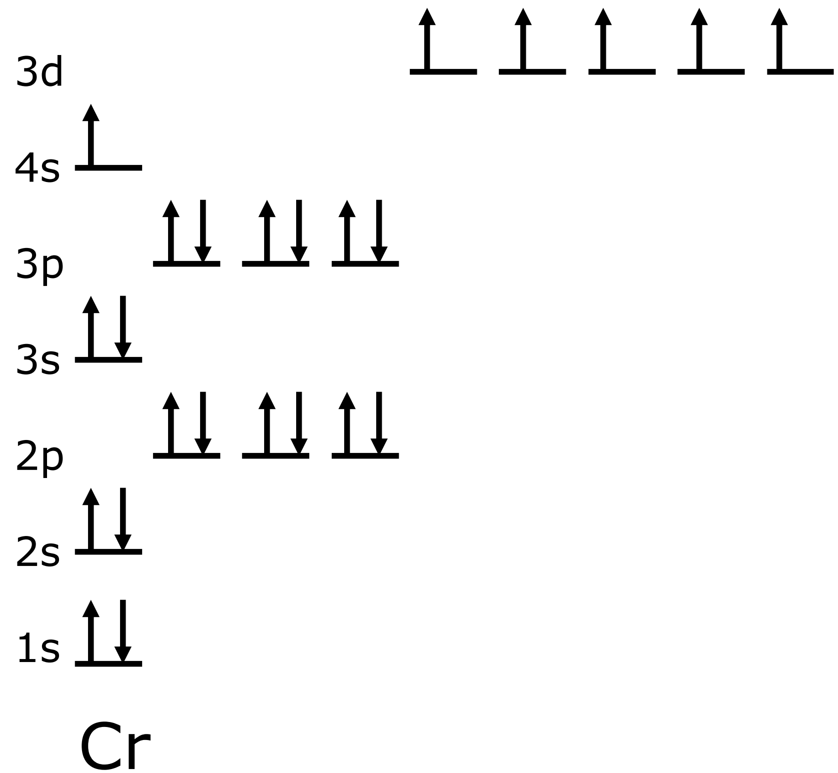
Exceptions to Aufbau Principle:

Example: chromium

Following the Aufbau Principle:



What actually happens:

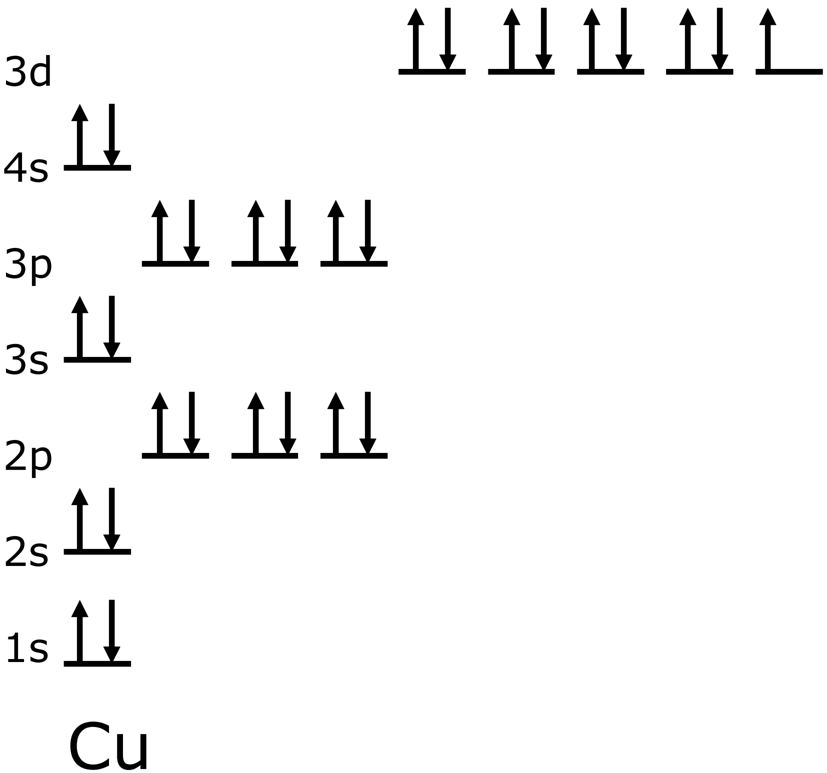


EXCEPTIONS TO AUFBAU PRINCIPLE

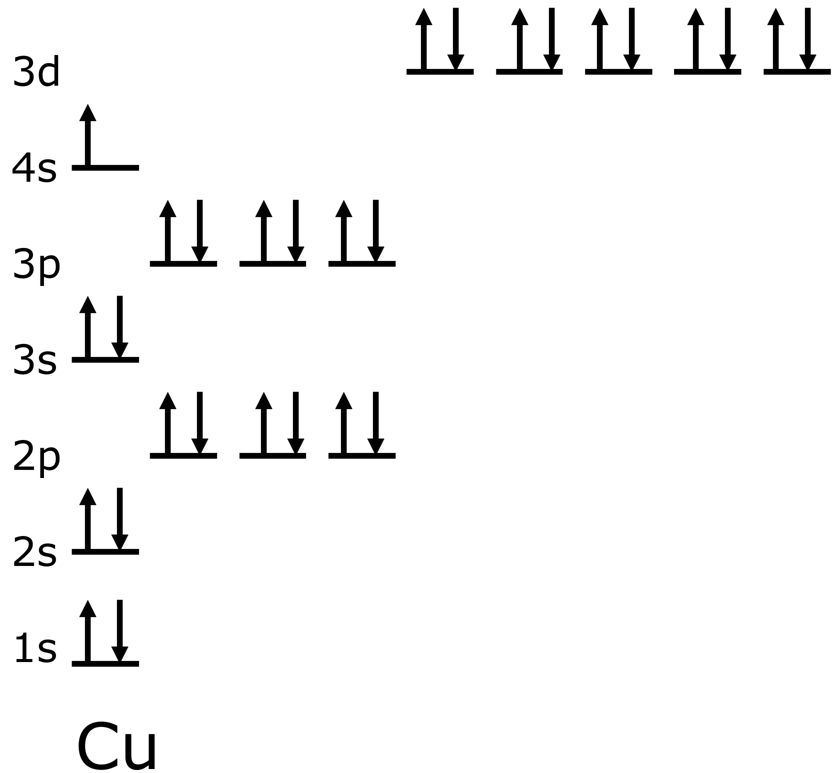
Exceptions to Aufbau Principle:

Example: copper

Following the Aufbau Principle:



What actually happens:



EXCEPTIONS TO AUFBAU PRINCIPLE

Why do these exceptions exist?

Experimental evidence indicates unfilled subshells are less stable than half-filled & filled subshells (have higher energy)

Filled and half-filled subshells have a lower energy state & are more stable

Filled subshell:

The 4s orbital is destabilized, but now the entire 3d subshell is stable

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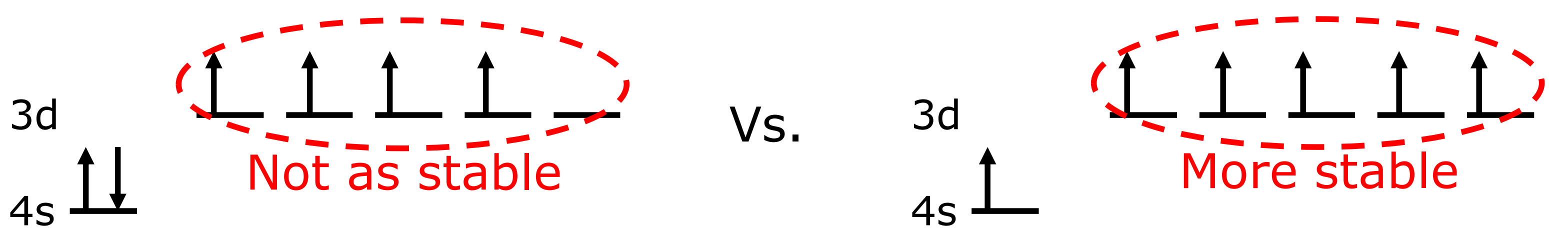
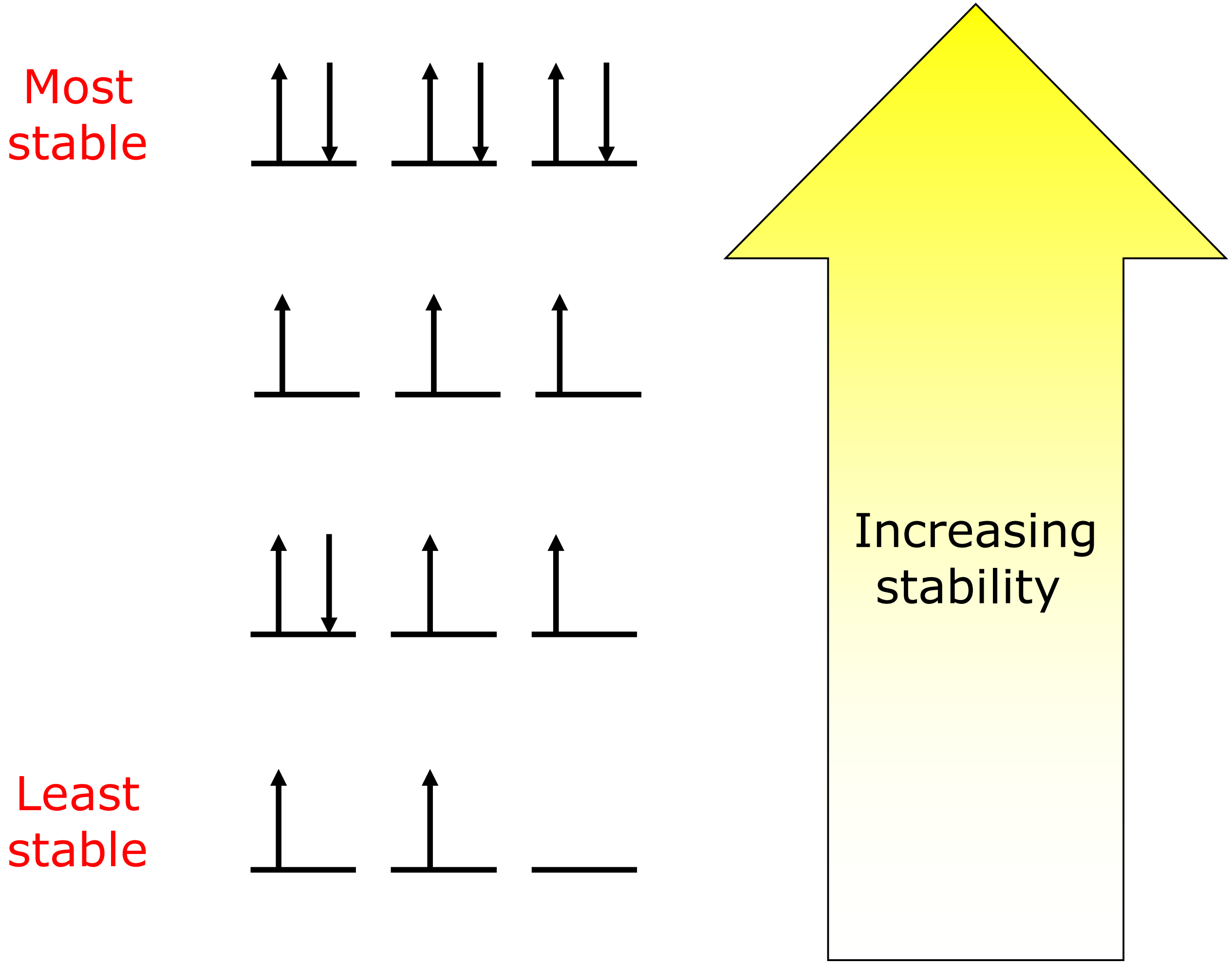
Half-filled subshell:



EXCEPTIONS TO AUFBAU PRINCIPLE

Stability: Rank the following from most to least stable

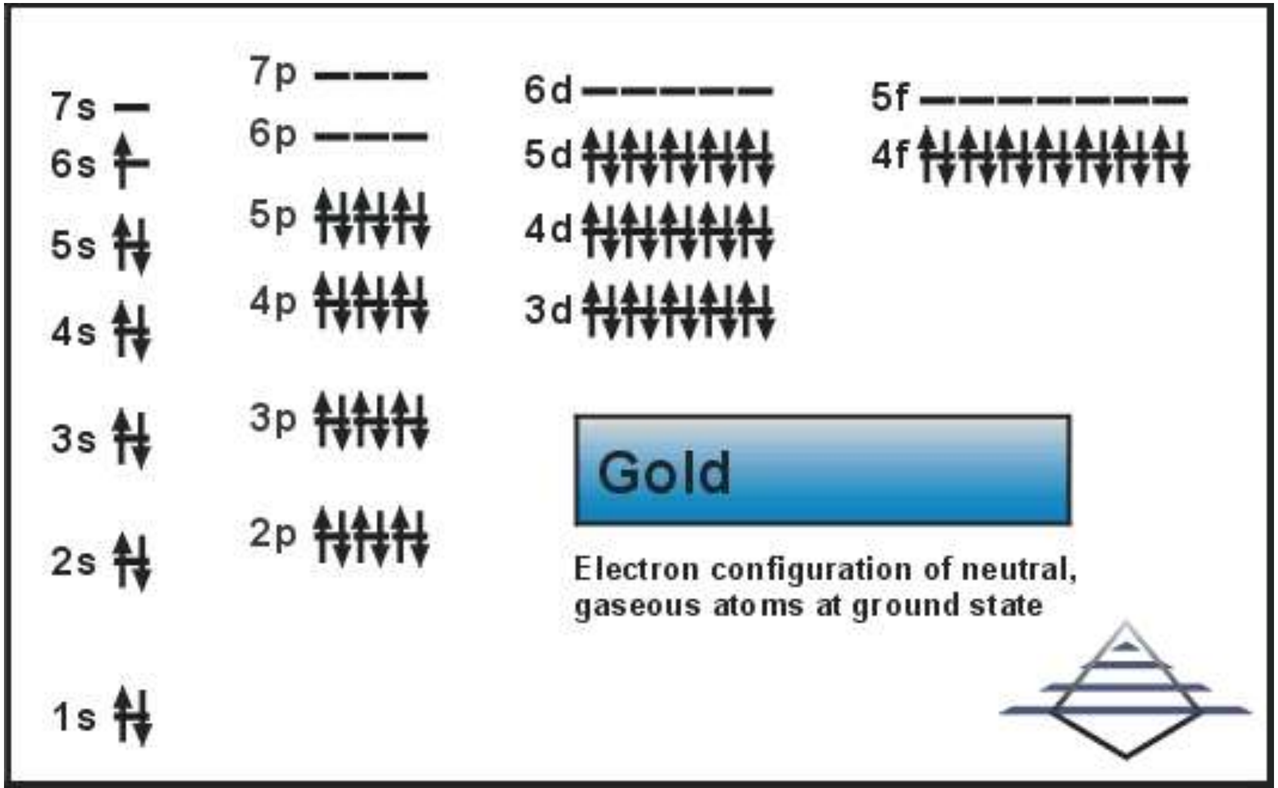


EXCEPTIONS TO AUFBAU PRINCIPLE

Working with exceptions:

Only use **d** orbitals where there is a possibility of moving an electron from an **s** to **d** orbital to achieve a half-filled or filled set of orbitals

Example: Au

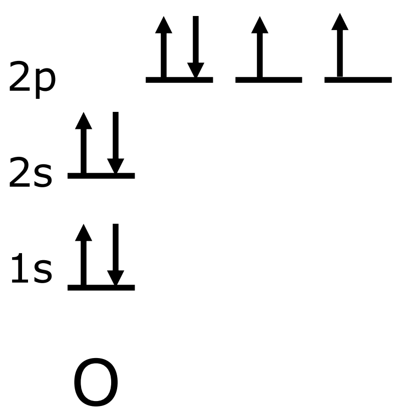


ELECTRON CONFIGURATIONS

Writing Electron Configurations

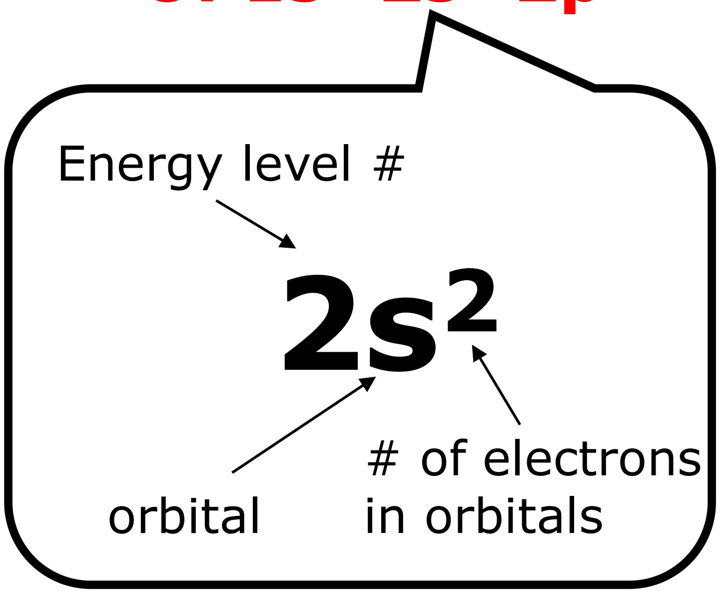
Electron configurations condense the information from electron energy-level diagrams

Electron energy level diagram



Electron configuration

O: $1s^2\ 2s^2\ 2p^4$



ELECTRON CONFIGURATIONS

Writing Electron Configurations

Electron configurations:

Cl:

Sn:

S^{2-}:

Fe:

ELECTRON CONFIGURATIONS

Writing Electron Configurations

Shorthand form of Electron configurations:

Cl: $\underbrace{1s^2\ 2s^2\ 2p^6}_{\text{Same configuration as Neon}}\ 3s^2\ 3p^5$

Cl:

Sn: $\underbrace{1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6}_{\text{Same configuration as krypton}}\ 5s^2\ 4d^{10}\ 5p^2$

Sn:

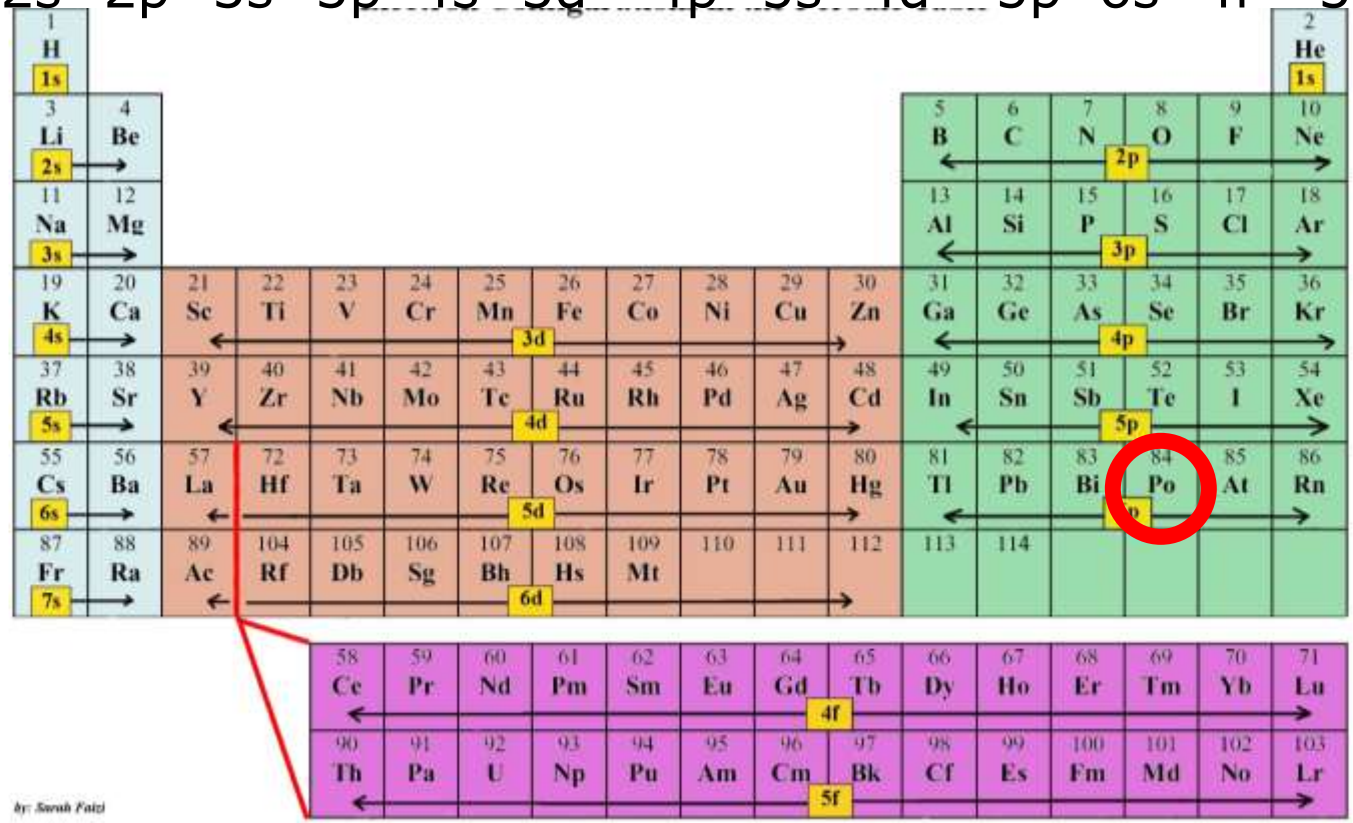
In the shorthand version, the "core electrons" of an atom are represented by the preceding noble gas

ELECTRON CONFIGURATIONS

Writing Electron Configurations

Identify the element that has the following electron configuration:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f^{14}\ 5d^{10}\ 6p^4$



It is the 4th element from the left

It is polonium (Po)

ELECTRON CONFIGURATIONS

Explaining multivalent metals:

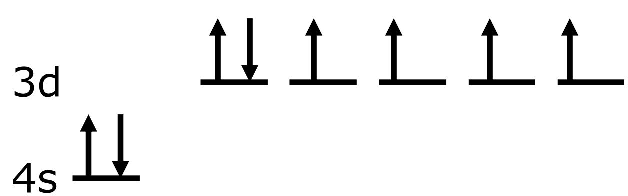
Electrons are lost to achieve stability:

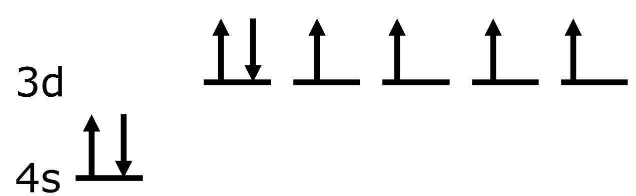
Cd: $[Kr]5s^{2}4d^{10}$ becomes Cd^{2+}

We can now explain why some transition metals can form multiple ions:

Pb: $[Xe]6s^{2}4f^{14}5d^{10}6p^{2}$ becomes Pb^{2+} or Pb^{4+}

Fe: $[Ar]4s^{2}3d^{6}$ becomes Fe^{2+} or Fe^{3+}





ELECTRON CONFIGURATIONS

Homework:

-Read page 171 on magnetism

- Complete page 172 #3 and 10