Chapter 9

Electrons in Atoms and the Periodic Table

- To understand the Periodic Table, we need to understand atoms

- To understand atoms, we need to understand the nature of matter at very very small length scales.

- Quantum Mechanics rules the very very small length scales.
  - But its effects definitely show up at large length scales

Quantum Mechanics is weird and counterintuitive.

The world at atomic and sub-atomic scale is sort of like Alice in Wonderland

Wave-particle duality

Matter is made of particles

but …

Particles can also act as waves. The smaller and lighter they are, the more wave-like they are.

We cannot understand matter at atomic scale without understanding waves

Waves

- Most waves involves the propagation of a disturbance in a medium.

- Water waves propagate by the up-down motion of water.

- Sound waves propagate by the rapid compression-decompression of air (or the liquid or solid through which they are traveling).

Light is also a wave. It is a form of electromagnetic wave (“electromagnetic radiation”).

Electromagnetic waves do not need a medium to travel. They kind of carry themselves through space!

All waves are characterized by

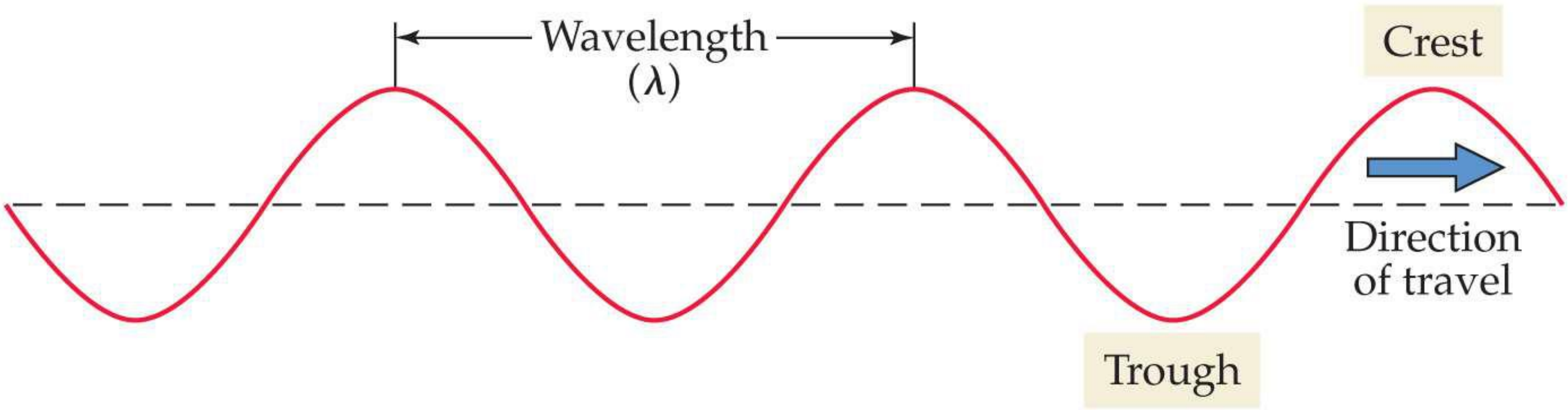
- **Wavelength (λ)** – distance between two consecutive peaks or troughs in a wave.
- **Frequency (ν)** – number of waves (cycles) per second that pass a given point in space
  - Frequency has the unit of inverse time (say, s^{-1})

    s^{-1} = “Hertz” (Hz)
  - “counts” or “number of waves” is not a physical unit
- **Speed (v)** – speed of propagation

Wavelength

Symbol: **λ** (lambda)

The distance between adjacent wave crests (or troughs, or any two equivalent points).

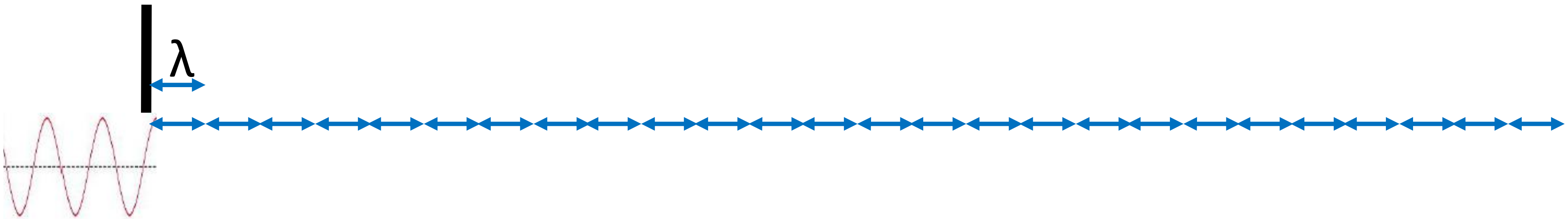


Frequency

Symbol: ν (“nu”) (yes, not “vee”)

Number of waves passing through a point per unit of time

Observing a sound wave for 1 second



26 waves (each 13.2 m in length) passed in 1 second

→ frequency = 26 s^{-1}

Wave speed = (number of waves per second)(length of each wave)

$$\overbrace{\text{Distance travelled in 1 sec.}}^{\text{Wave speed}} = \overbrace{26\text{ wave/s}}^{\nu}\ \text{x}\ \overbrace{13.2\text{ m/wave}}^{\lambda} = 343\text{ m/s}$$

$$\text{Wave speed} = \nu\,\lambda$$

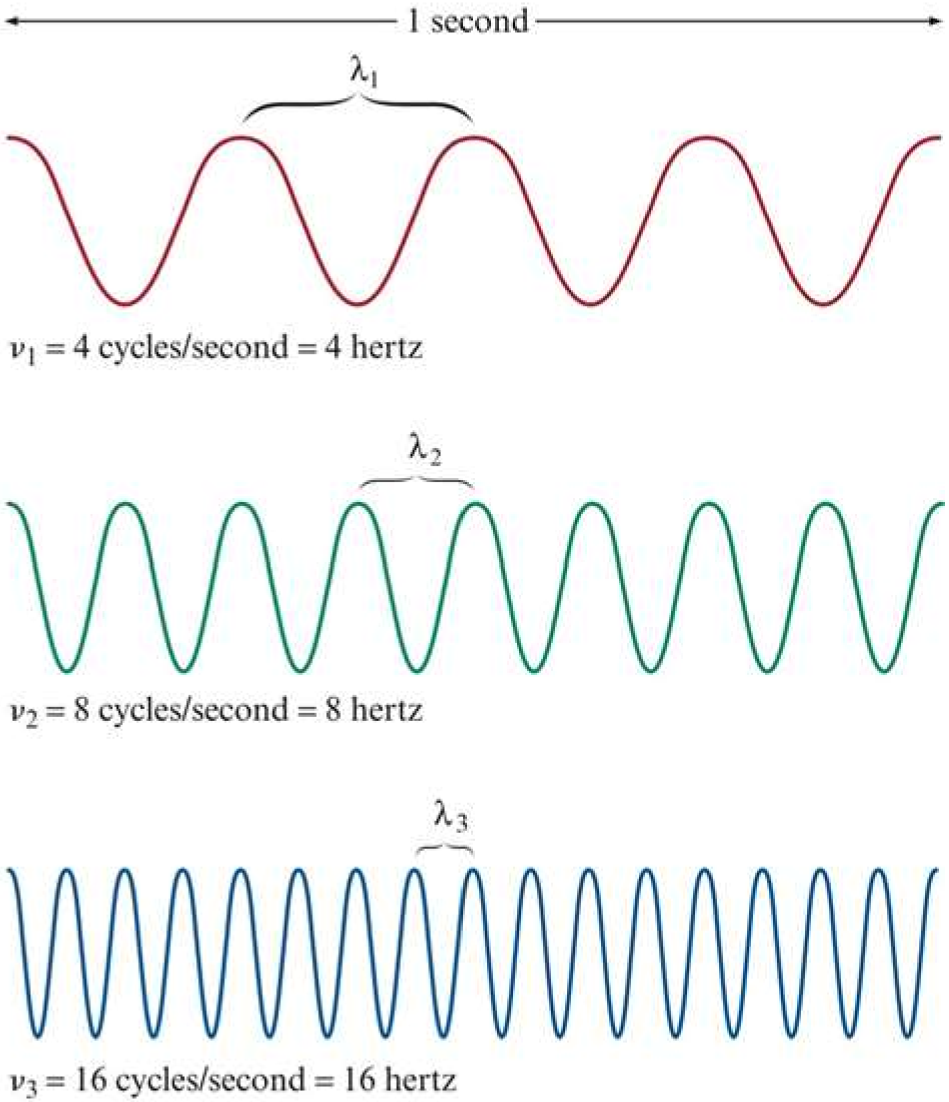
$$v = \lambda \nu$$

- Make sure you use consistent units.
- If v is in m/s, λ should be in m (not, say, in nm)
- If v is in km/hours, λ should be in km and

  ν should be in hours^{-1}

Frequency and wavelength are inversely related

Lower frequency
Longer wavelength



Higher frequency
Shorter wavelength

For electromagnetic radiation (including light):

$$\boxed{c = \nu \lambda}$$

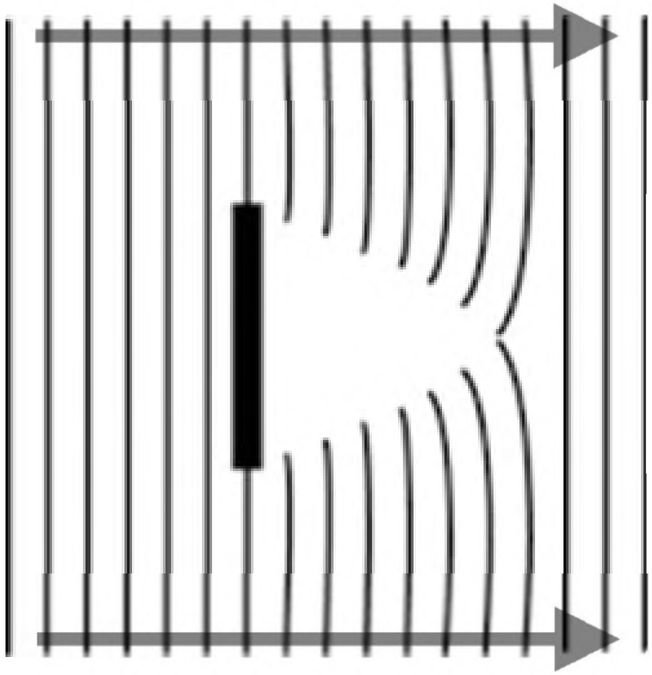
Speed of light

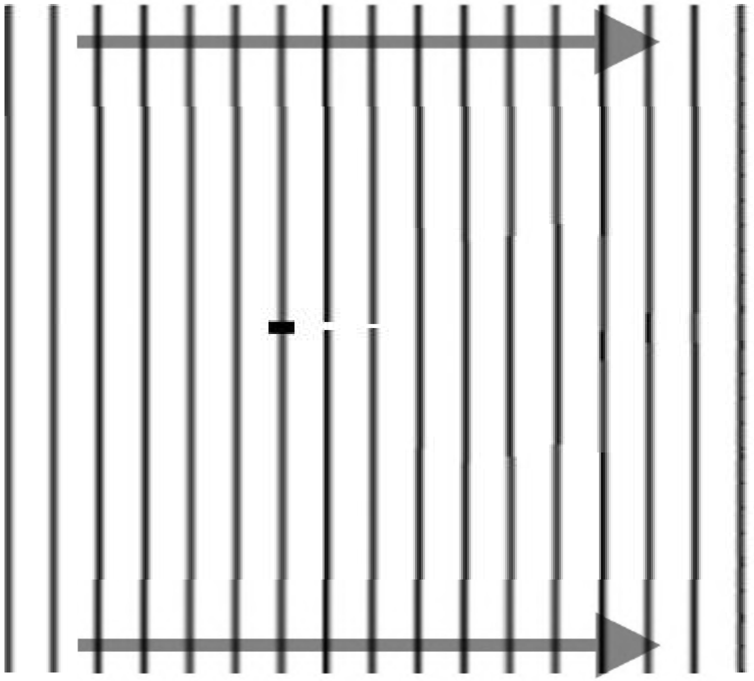
c = speed of light (2.9979×10^8 m/s)

Waves diffract

Waves bend around obstacles.

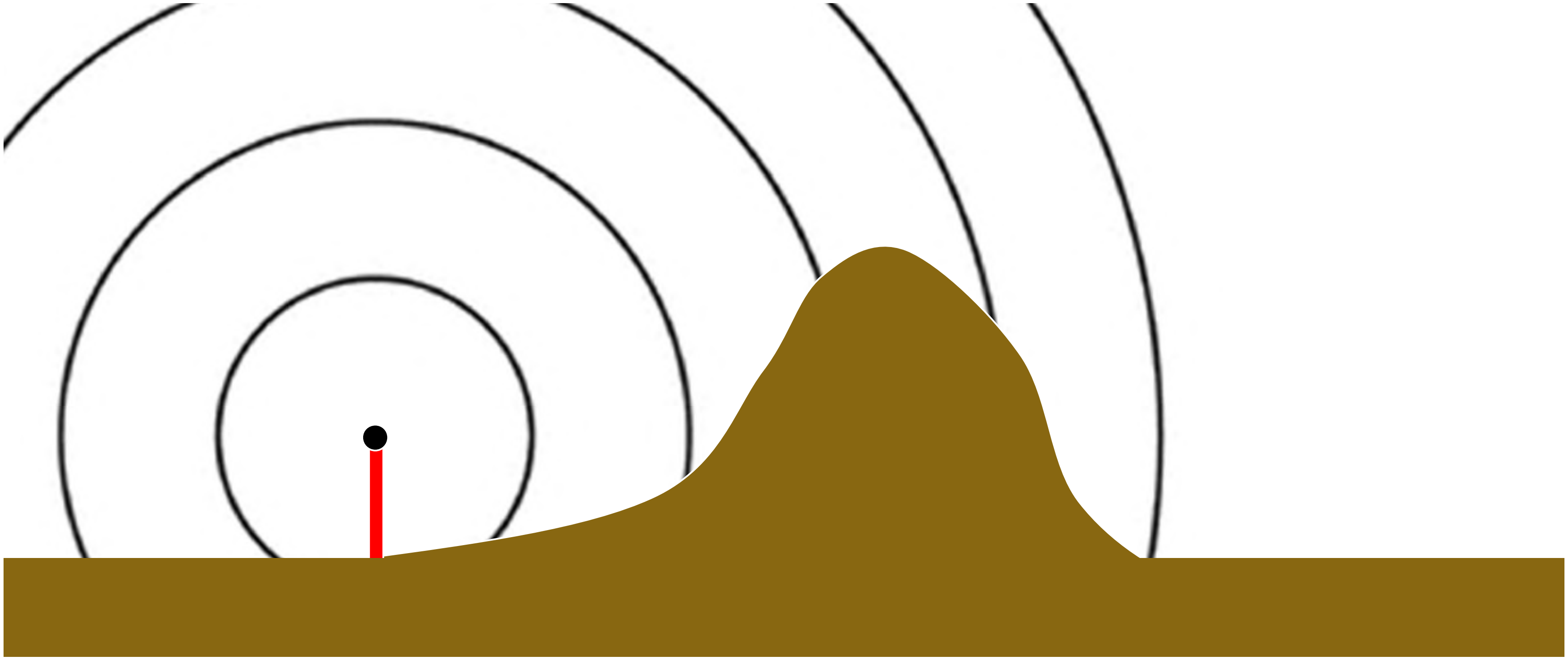
Moving into the region where there was supposed to be a “shadow”





If the obstacle is a lot smaller than the wavelength, it’s basically “invisible” to the wave

- To observe appreciable diffraction, wave length should not be much smaller than the feature it encounters
- Otherwise, only a tiny fraction of the wave would bend and diffract, i.e. “act like a wave”



Radio waves with long wavelengths can be received behind hills, but shorter wavelengths can’t.

- To observe appreciable diffraction, wave length should not be much smaller than the feature it encounters
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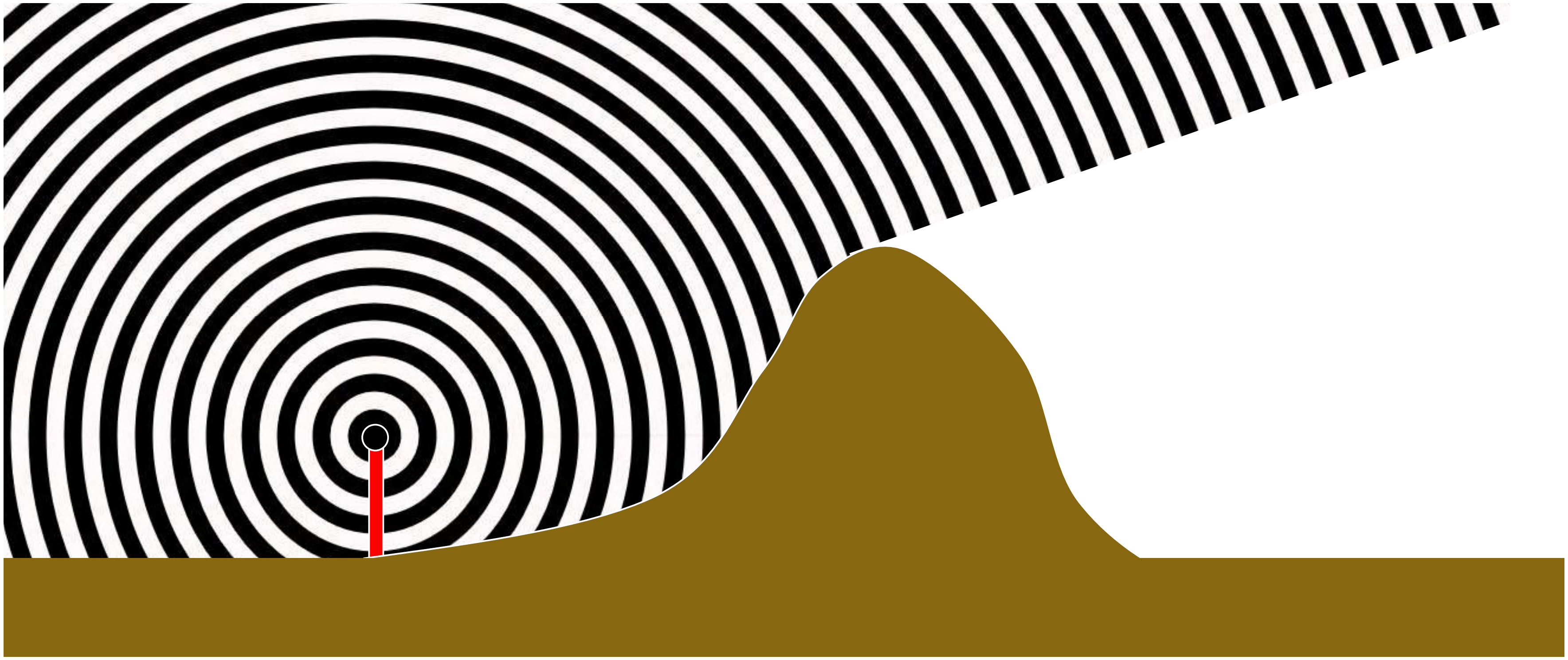
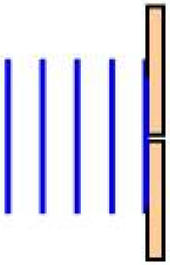
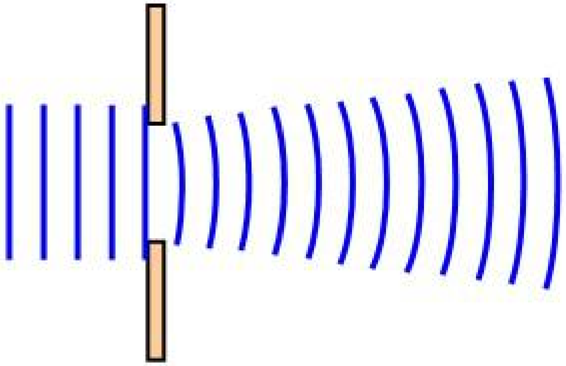


Radio waves with long wavelengths can be received behind hills, but shorter wavelengths can’t.

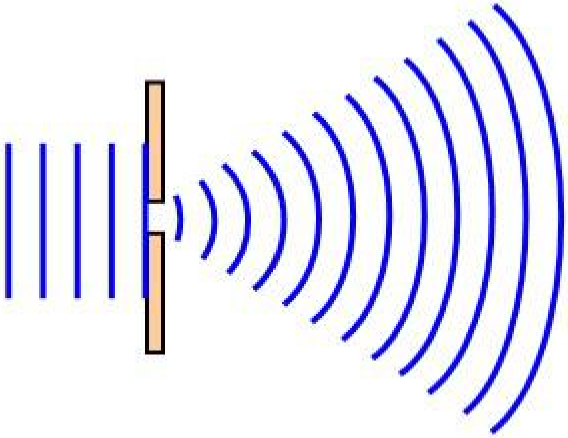
If a hole is much smaller than the wavelength, it’s blocked
-- it can’t “see” the hole



If a hole is much larger than the wavelength, the diffraction (the bending effect) will be small.

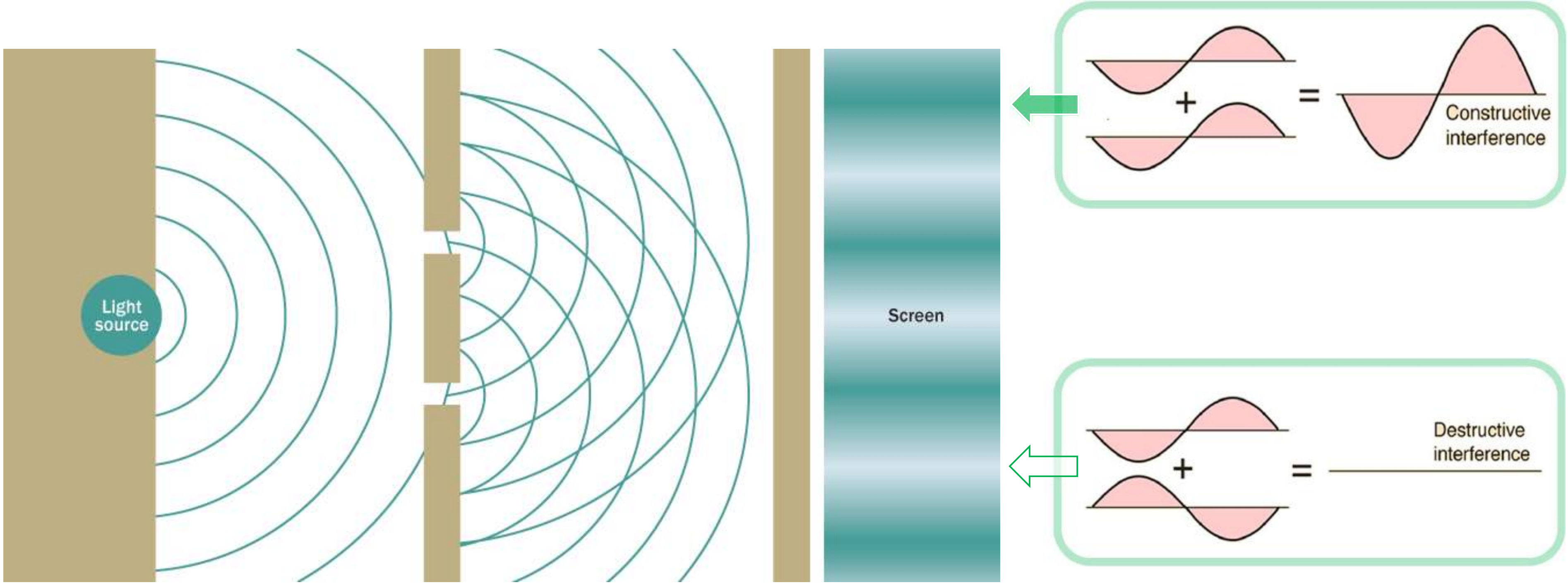


If a hole is about the same size as the wavelength, it will act as a **point source** (waves will come out of it, with the hole at the center)



Waves on water diffract too!

Diffraction by multiple features cause “interference”



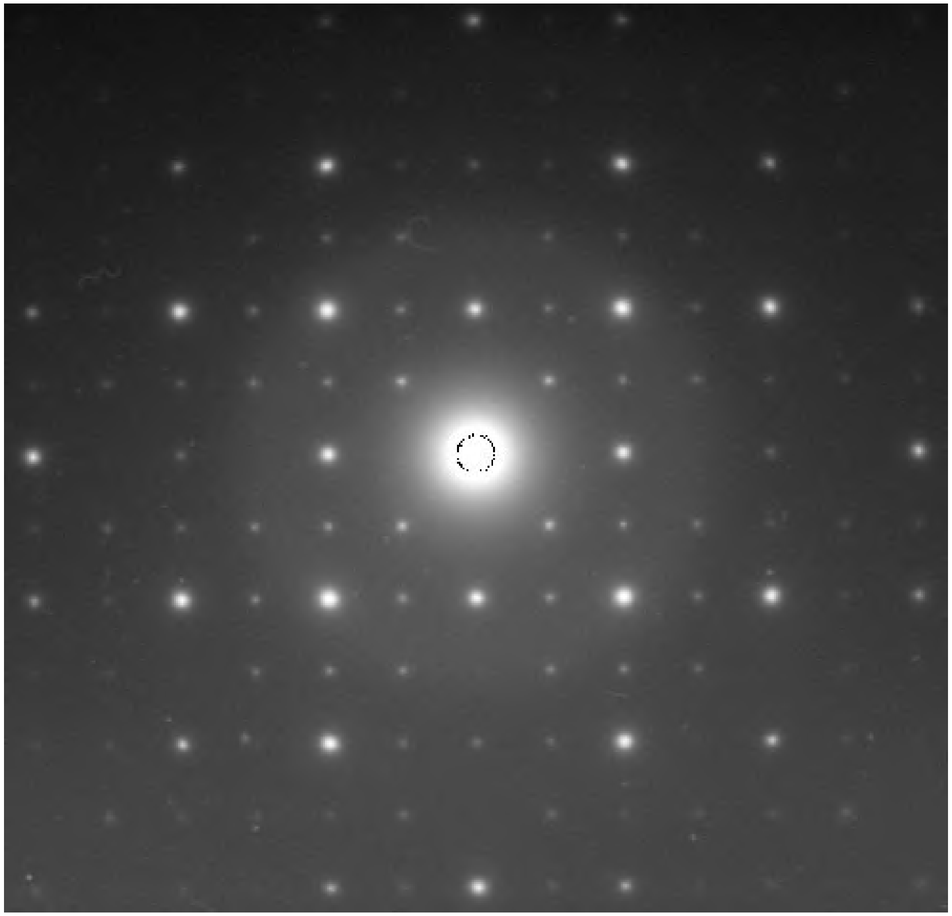
E. Otwell, sciencenews.org

Diffraction by multiple features cause “**diffraction interference**”

- Where wave peaks coincide, amplitudes add up
- Where a wave peak coincides with another wave’s trough, amplitudes cancel
- Creating an “interference pattern”

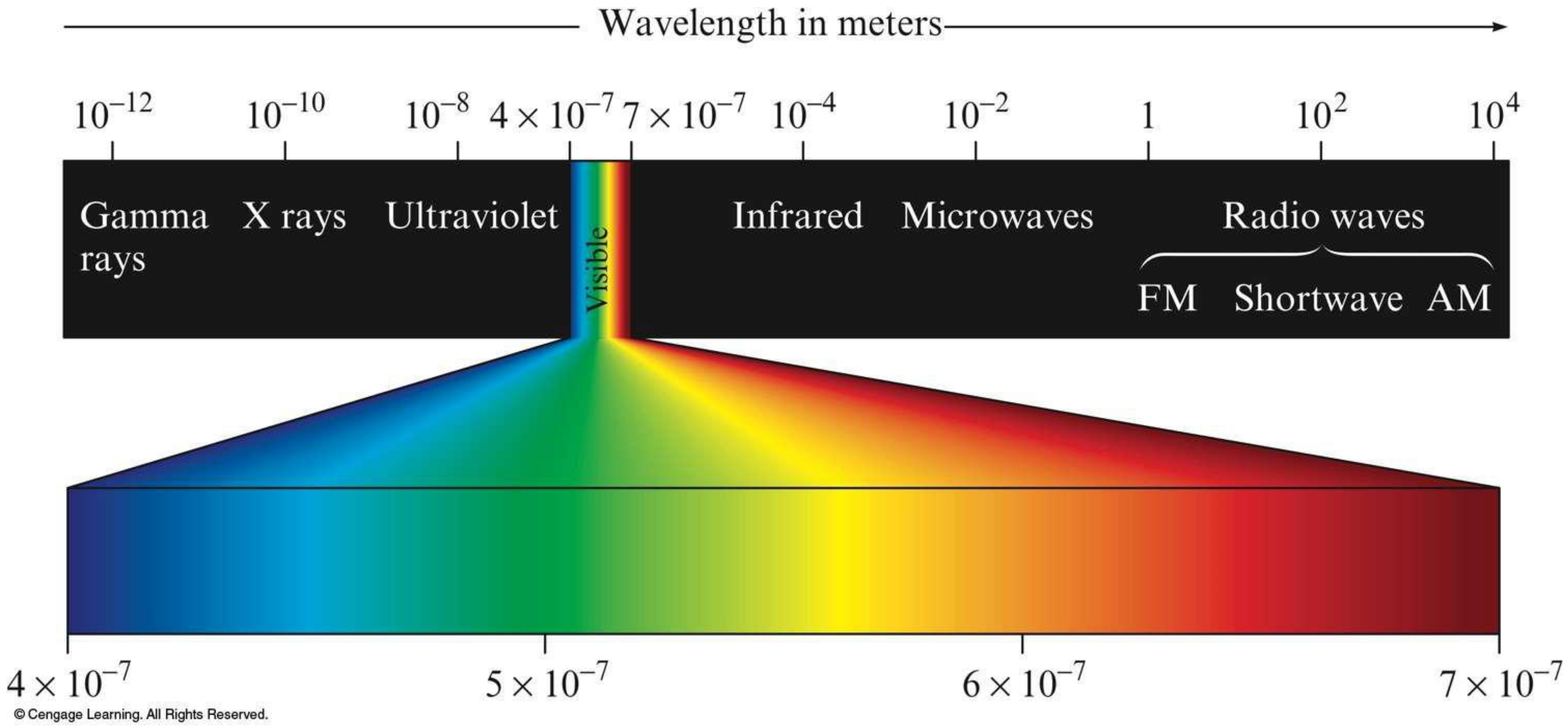
Diffraction of X-rays by atoms in a crystal lattice also form a diffraction pattern

Distance ("hole") between atoms : Angstroms (10^{-10} m)
X-ray wavelengths: Angstroms (10^{-10} m)



Crystal structures and structures of molecules in a crystal are discovered by analyzing the X-ray diffraction patterns

Classification of Electromagnetic Radiation



400 nm

700 nm

We said earlier:

Electromagnetic waves do not need a medium to travel. They kind of carry themselves through space!

- That's because they also are "particles", called photons.
- Photons are basically a "packet" of energy.
- A photon has no "rest mass". Its mass is due to its energy, because $E=mc^2$
- We cannot stop a photon. If we could, it would have no mass.
- Put another way, if we "stop" a photon it gives up its energy, and therefore its mass. It disappears.

So,

- **Electromagnetic radiation** exhibits wave properties <u>and</u> particulate properties.

It’s much more than an “example”:

- Its fundamental properties led to the leaps of intuition that developed Quantum Mechanics
  - Wave-particle duality extended to all matter
- And its essential role in an atom’s gaining or losing energy allow the actual measurements of energy changes

Light

It turns out that the energy of a photon is directly proportional to frequency of the light.

$$E_{photon} = h\upsilon = \frac{hc}{\lambda}$$

Planck's constant = h= 6.626 × 10^{-34} J.s

- Energy can be gained or lost only in whole number multiples of $h\nu$
- A system can transfer energy only in whole quanta (or “packets”)

Photoelectric effect showed that photons transfer all of their energy or none at all

Electrons are emitted from a metal’s surface when struck by light

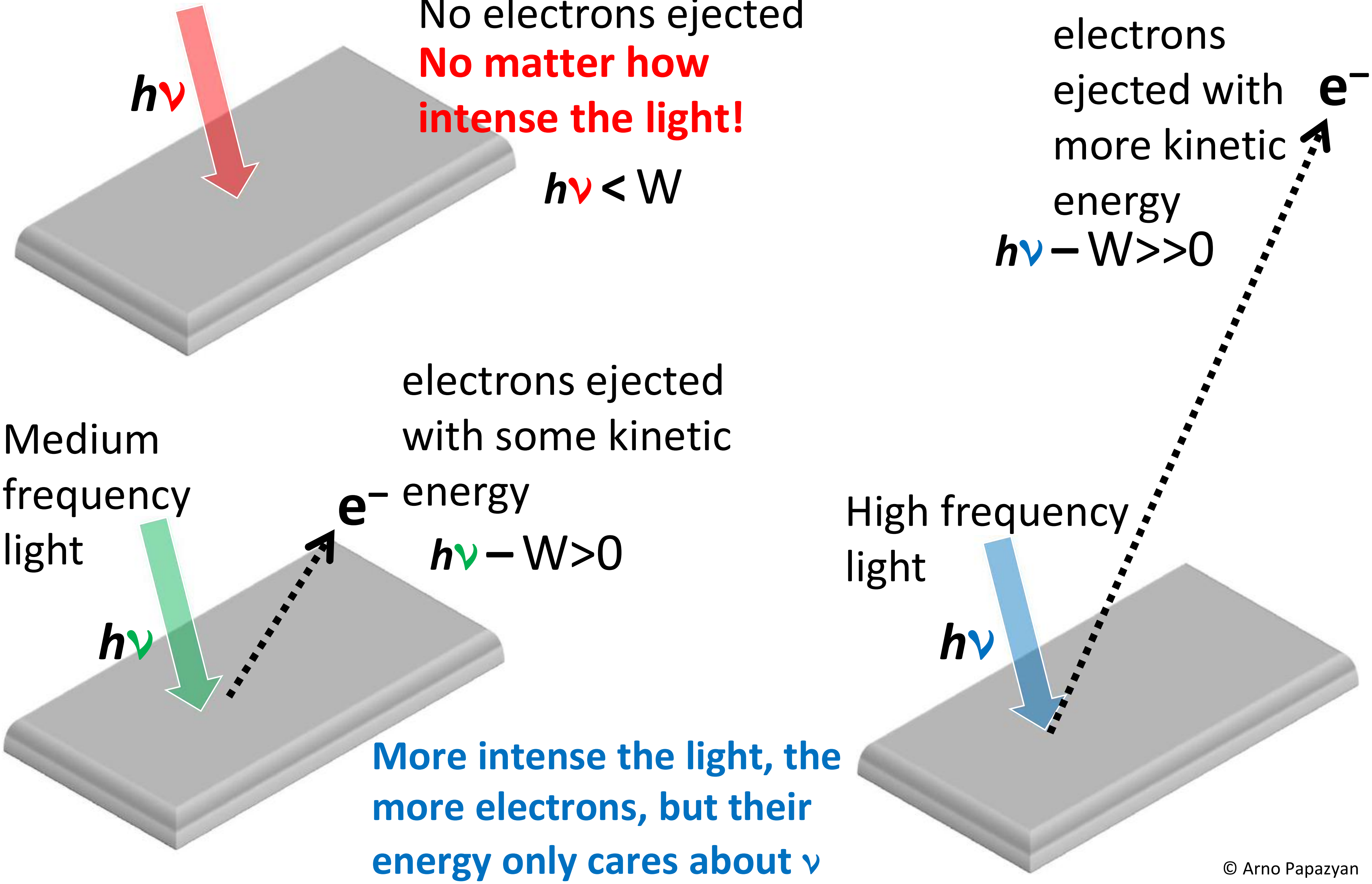
Kinetic energy of ejected electron = $\boldsymbol{h\nu} - W$

Photon energy

Photon energy required to remove the electron from the metal’s surface

If the energy of the photon is less than the threshold W, electrons are not emitted, <u>no matter how many photons we send</u>.

Photoelectric effect



Low frequency light

No electrons ejected

No matter how intense the light!

$h\nu < W$

electrons
ejected with
more kinetic
energy

$h\nu - W >> 0$

Medium
frequency
light

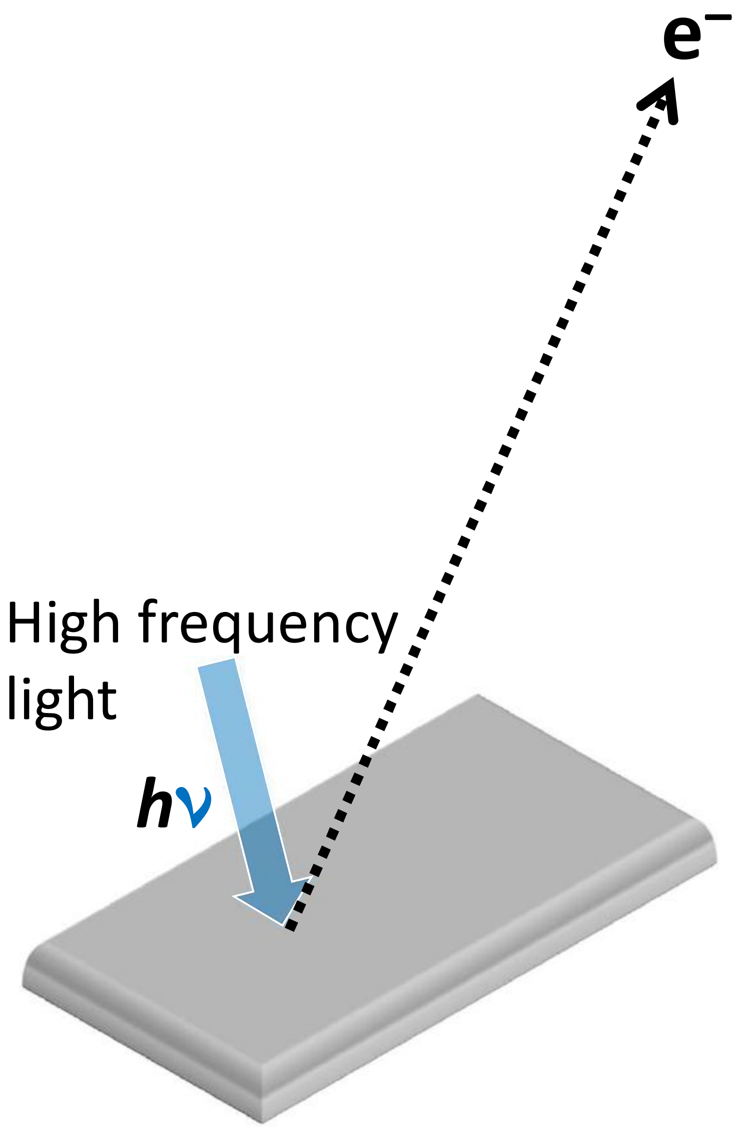
electrons ejected
with some kinetic
energy

$h\nu - W > 0$

High frequency
light

More intense the light, the more electrons, but their energy only cares about ν

Photoelectric effect



Leftover energy

$$\text{kinetic energy of } \mathbf{e}^- = h\nu - W$$

Energy brought by the photon

Energy spent to break away from the metal surface

Einstein explained the photoelectric effect:

- Light is made of individual energy “quanta”
  - Called **photons**
- Each photon carries a quantity of energy proportional to the frequency of light

$$E_{photon} = h\nu$$

$h = 6.626 \times 10^{-34}$ J·s Planck’s constant

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Why not "Einstein's constant"?

- Max Planck had theorized that the energy gained or lost via light was proportional to the light frequency ($|\Delta E| = h\nu$), to explain the light emitted by objects at a given temperature, but was not convinced that it corresponded to anything real.
- Einstein's explanation of photoelectric effect made it clear it was real.

Photon’s discovery allowed us to know:

- The “currency” of energy exchange involving electromagnetic radiation: photon
- The energy value of that “currency” (by measuring frequency or wavelength)
- We then knew that a light of certain frequency corresponded to an energy loss of that exact same energy by *something*

$$E_{photon} = |\Delta E| = h\nu$$

Practice:

Check your solution on next page

Calculate the number of photons in a laser pulse with wavelength 337 nm and total energy 3.83 mJ

Practice: Calculate the number of photons in a laser pulse with wavelength 337 nm and total energy 3.83 mJ

Given: λ = 337 nm, E_{pulse} = 3.83 mJ

Find: number of photons

Conceptual Plan:

$$\lambda(\text{nm}) \xrightarrow[\frac{10^{-9}\text{ m}}{1\text{nm}}]{} \lambda\ (\text{m}) \xrightarrow[E_{\text{photon}} = \frac{hc}{\lambda}]{} E_{\text{photon}} \xrightarrow[\frac{E_{\text{pulse}}}{E_{\text{photon}}}]{} \text{number photons}$$

Relationships: $E=hc/\lambda$, 1 nm = 10^{-9} m, 1 mJ = 10^{-3} J, $E_{\text{total}}=E_{\text{photon}} \bullet$ # photons

Solve:

$$3.37\times10^{2}\ \cancel{\text{nm}}\times\frac{10^{-9}\text{ m}}{1\cancel{\text{nm}}} = 3.37\times10^{-7}\text{ m}$$

$$E_{\text{photon}} = \frac{hc}{\lambda} = \frac{(6.626\times10^{-34}\text{ J}\bullet\cancel{\text{s}})(3.00\times10^{8}\ \cancel{\text{m}}\bullet\cancel{\text{s}^{-1}})}{3.37\times10^{-7}\ \cancel{\text{m}}} = 5.8\underline{9}85\times10^{-19}\text{ J}$$

$$3.83\ \cancel{\text{mJ}}\times\frac{10^{-3}\text{ J}}{1\cancel{\text{mJ}}} = 3.83\times10^{-3}\text{ J}$$

$$\boxed{\begin{aligned}\text{number of photons} &= \frac{3.83\times10^{-3}\ \cancel{\text{J}}}{5.8\underline{9}85\times10^{-3}\ \cancel{\text{J}}}\\ &= 6.49\times10^{15}\text{ photons}\end{aligned}}$$

Practice:

Check your solution on next page

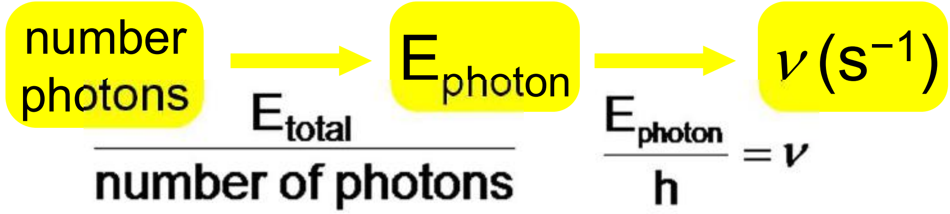
What is the frequency of radiation required to supply 1.0×10^2 J of energy from 8.5×10^{27} photons?

Practice – What is the frequency of radiation required to supply 1.0 x 10^2 J of energy from 8.5 x 10^{27} photons?

Given: E_{total} = 1.0 x 10^2 J, number of photons = 8.5 x 10^{27}

Find: ν

Conceptual Plan:



$$\begin{tikzcd} \text{number photons} \arrow[r, "\frac{E_{total}}{\text{number of photons}}"'] & E_{photon} \arrow[r, "\frac{E_{photon}}{h} = \nu"'] & \nu\,(s^{-1}) \end{tikzcd}$$

Relationships: E=hν, $E_{total} = E_{photon} \cdot \#$ photons

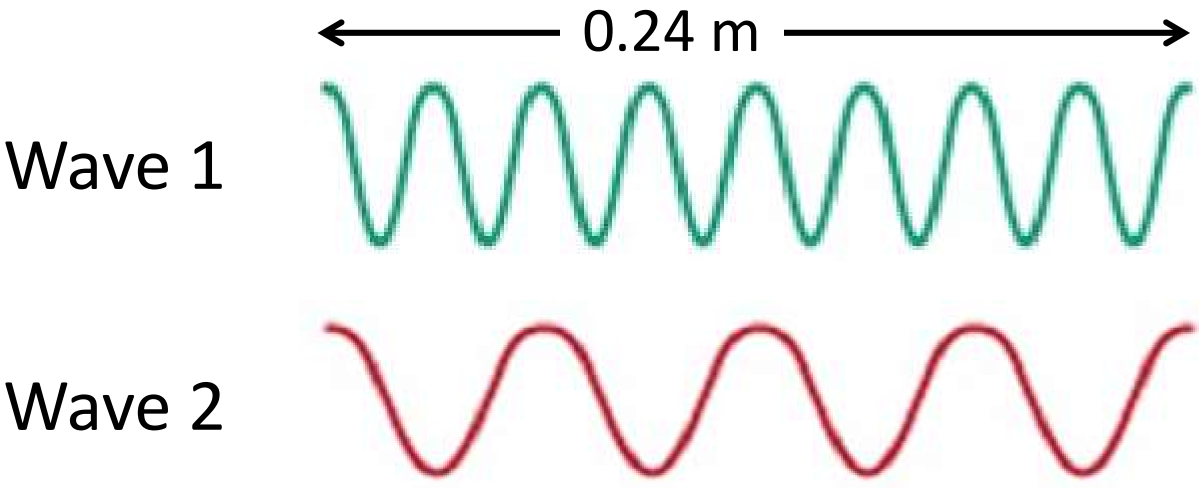
Solve:

$$E_{photon} = \frac{1.0 \times 10^2\ \text{J}}{8.5 \times 10^{27}} = 1.\underline{1}76 \times 10^{-26}\ \text{J}$$

$$\nu = \frac{E_{photon}}{h} = \frac{\left(1.\underline{1}76 \times 10^{-26}\ \cancel{\text{J}}\right)}{6.626 \times 10^{-34}\ \cancel{\text{J}} \bullet \text{s}} = 1.8 \times 10^{7}\ \text{s}^{-1}$$

Practice:
Check your solution on next page

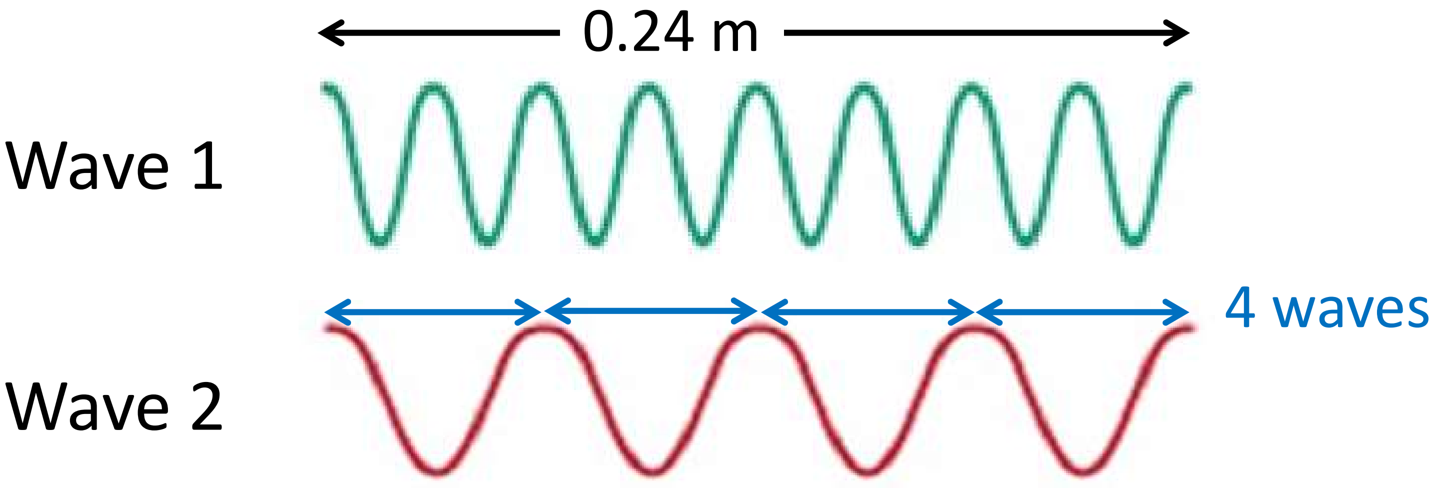
Consider two different electromagnetic waves:



Which wave has the longer wavelength? What is its wavelength? What is its frequency?

Practice

Consider two different electromagnetic waves:



Which wave has the longer wavelength? What is its wavelength? What is its frequency?

Wavelength(λ) = (0.24 m)/4 = 0.060 m = 6.0 cm

Frequency(ν) = c/ λ = (3.00×10^{8}m s^{-1})/(0.060 m) = 5.0×10^{9} s^{-1} (Hz)

Practice , Check your solution on the next page

One electromagnetic radiation (let's call it EM1) has a:
frequency of 89.3 MHz

A second electromagnetic radiation (EM2) has a:
wavelength of 31.0 meters

A third electromagnetic radiation (EM3) has a:
photon energy of 4.42x10^{-19} Joules

Sort EM1, EM2, and EM3 in increasing order of photon energy.

Practice

One electromagnetic radiation (let's call it EM1) has a:
frequency of 89.3 MHz (Hz = s^{-1} ; MHz = 10^6 Hz = 10^6 s^{-1})

A second electromagnetic radiation (EM2) has a:
wavelength of 31.0 meters

A third electromagnetic radiation (EM3) has a:
photon energy of $4.42\text{x}10^{-19}$ Joules

Sort EM1, EM2, and EM3 in increasing order of photon energy.

EM1: $E_{photon} = h\nu = (6.626\text{x}10^{-34}\ \text{J}\cdot\text{s})(89.3\text{x}10^{6}\ \text{s}^{-1}) = 5.92\text{x}10^{-26}$ J

EM2: $E_{photon} = h\nu = hc/\lambda = (6.626\text{x}10^{-34}\ \text{J}\cdot\text{s})(3.00\text{x}10^{-8}\ \text{m/s}) / (31.0\ \text{m})$
$= 6.41\text{x}10^{-27}$ J

EM3: $E_{photon} = 4.42\text{x}10^{-19}$ J

EM2 , EM1 , EM3

Practice , Check your solution on the next page

What is the wavelength (in nm) of the highest-energy photon in the previous question?

Practice

What is the wavelength (in nm) of the highest-energy photon in the previous question?

$E_{photon} = 4.42\text{x}10^{-19}\ \text{J}$ $\quad E_{photon} = hc/\lambda \Longrightarrow \lambda = hc/\ E_{photon}$

$\lambda = (6.626\text{x}10^{-34}\ \text{J}\cdot\text{s})(3.00\text{x}10^{8}\ \text{m/s})\ /\ (4.42\text{x}10^{-19}\ \text{J}) = 4.50\text{x}10^{-7}\ \text{m}$

$\lambda = (4.50\text{x}10^{-7}\ \text{m})(1\ \text{nm}\ /\ 10^{-9}\ \text{m}) = 450.\ \text{nm}$

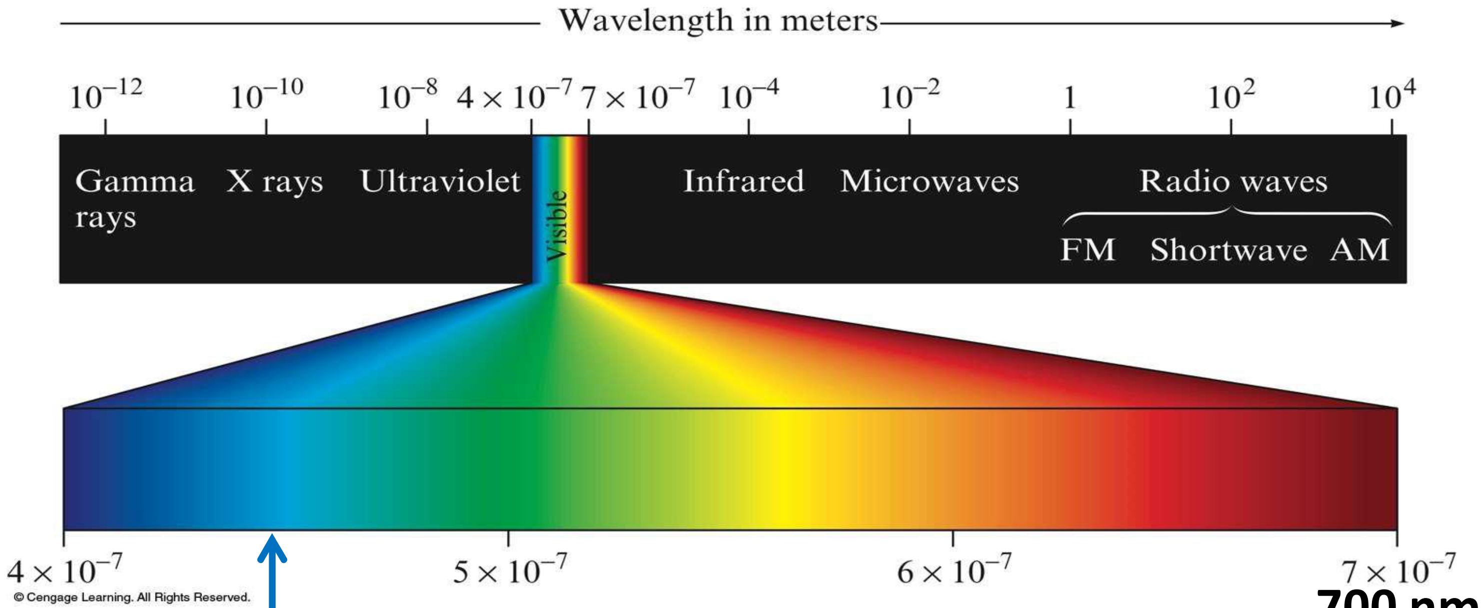
Practice , Check your solution on the next page

What region of the electromagnetic spectrum does this photon in the previous question belong to?

Practice

What region of the electromagnetic spectrum does this photon in the previous question belong to?

λ = 450. nm

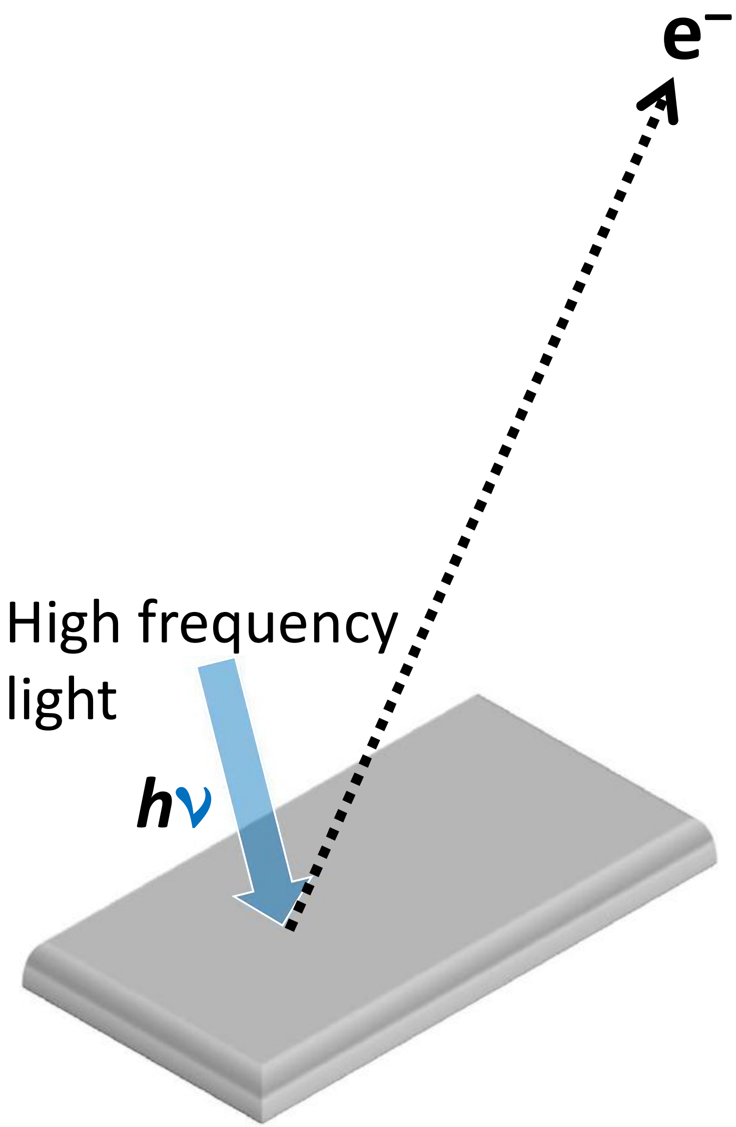


400 nm

700 nm

Visible; blue

For the practice on the next slide we remember Photoelectric effect



Leftover energy

kinetic energy of $\mathbf{e}^-$ = $h\nu$ − W

Energy brought by the photon

Energy spent to break away from the metal surface

Practice (Check your solution on the next page)

The energy (W) required to free an electron from the surface of solid Cesium metal is 3.37×10^{-19} J. Does the photon in the previous question have enough energy to display the photoelectric effect with Cesium? If so, what would be the kinetic energy the ejected electron?

Practice

The energy (W) required to free an electron from the surface of solid Cesium metal is 3.37×10^{-19} J. Does the photon in the previous question have enough energy to display the photoelectric effect with Cesium? If so, what would be the kinetic energy the ejected electron?

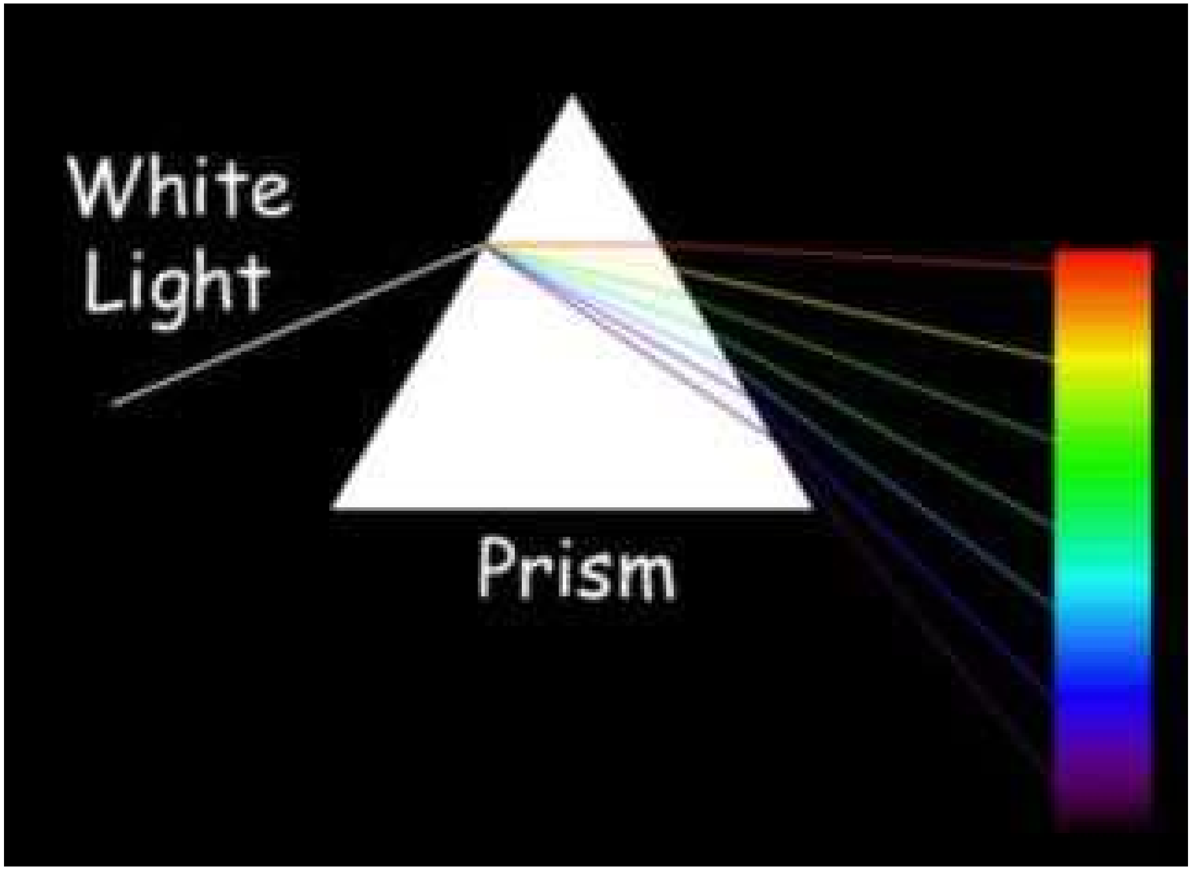
$$E_{photon} = 4.42 \times 10^{-19}\ J$$

$$E_{electron} = E_{photon} - W = (4.42 \times 10^{-19}\ J) - (3.37 \times 10^{-19}\ J) = 1.05 \times 10^{-19}\ J$$

Energy of the free electron is in the form of kinetic energy since it is freed from any forces, and is now moving in vacuum.

Sunlight contains a continuous distribution of light frequencies, corresponding to energies (therefore energies lost by emitting light)

An essentially infinite variety of processes fueled by thermal motions, emitting photons of **all the possible energies in and around the visible wavelength range**



(Image: © NASA)

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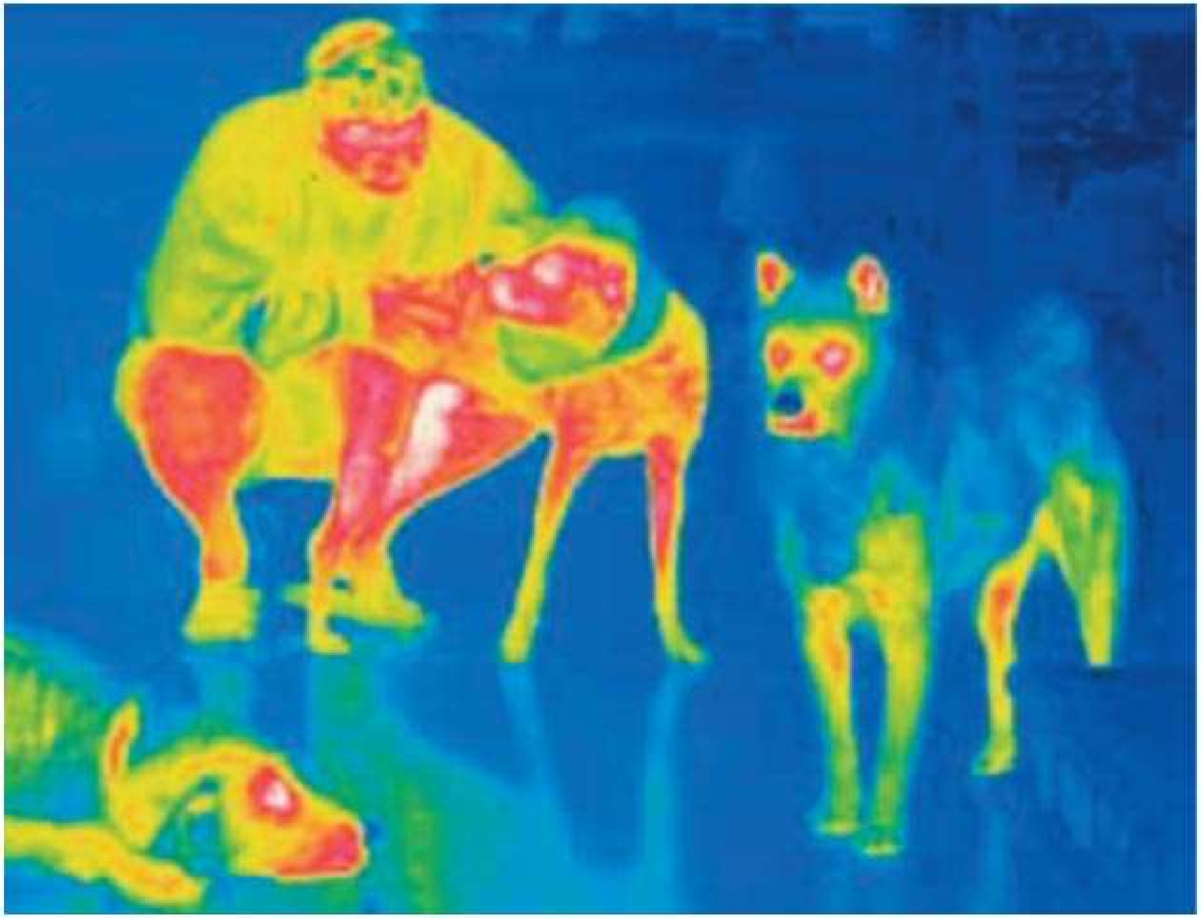
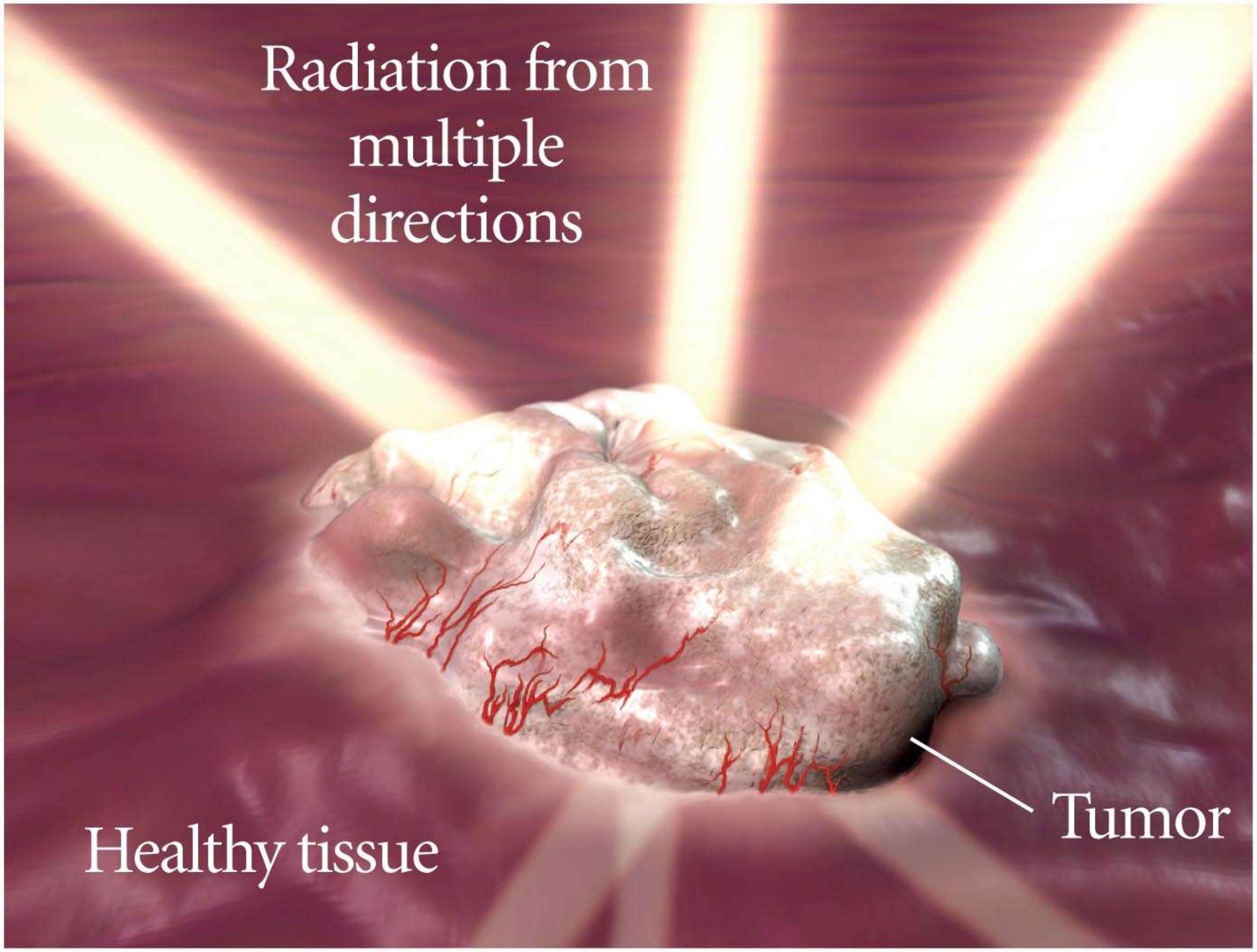
Thermal Imaging using Infrared Light



Sunburns Caused by High-Energy UV Radiation

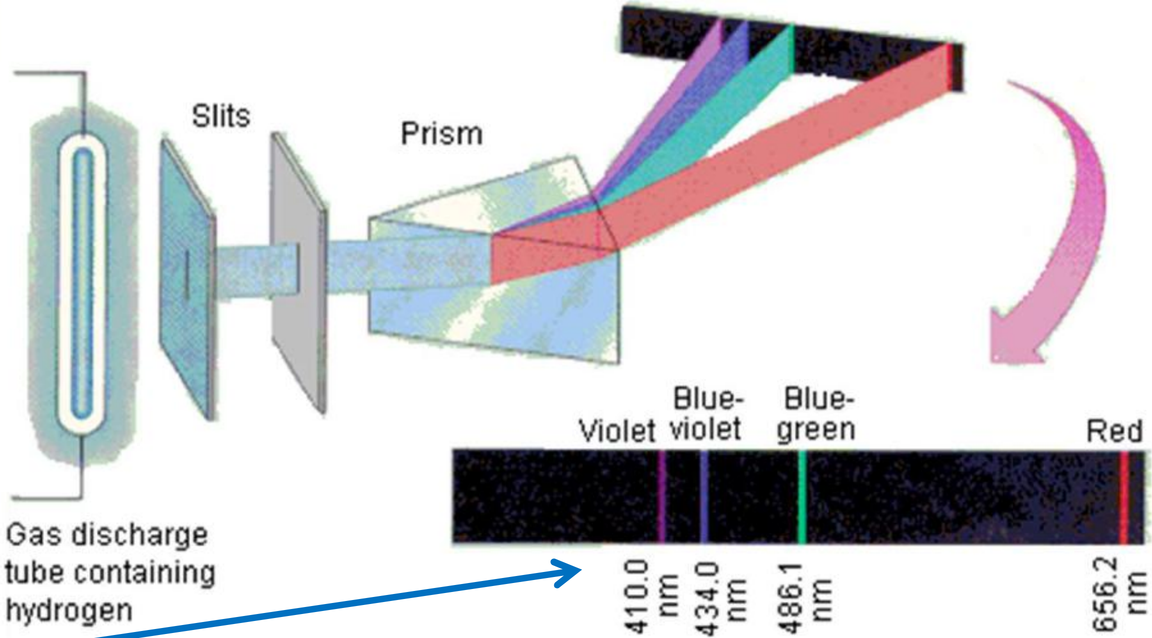
Using High-Energy Radiation to Kill Cancer Cells



- When atoms are given extra energy that makes them more energetic than their most stable, “ground” level, they eventually relax and lose the energy by emitting a photon.
- When “alone” in the gas phase, the only way to lose the extra energy is for an electron to go from a higher energy level to a lower level.

Hydrogen atoms in the gas phase emit light with **only several discrete wavelengths:**

“line spectrum”



http://chemed.chem.purdue.edu/genchem/topicreview/bp/ch6/bohr.html

The “line spectrum” of hydrogen, and gases of other elements, implied:

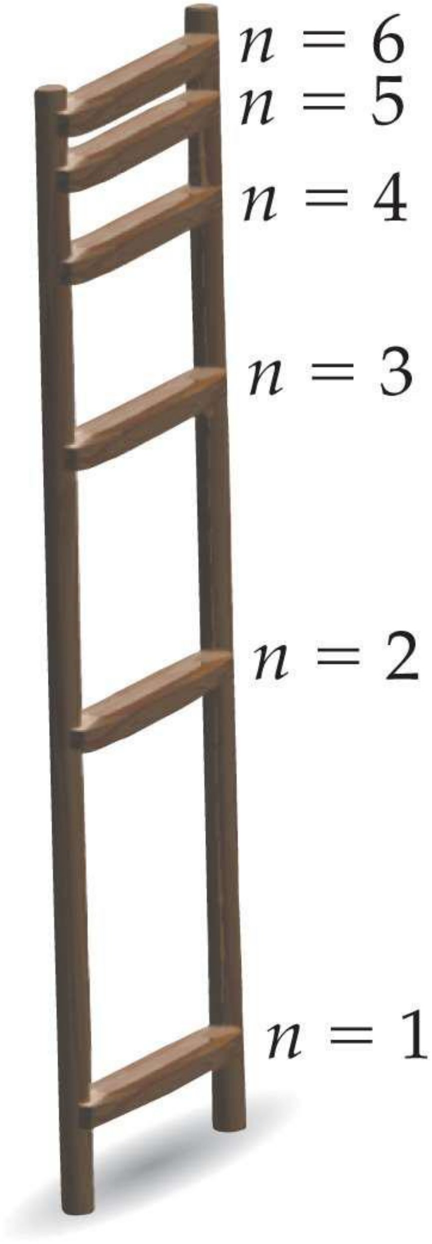
Since there are only certain ΔE values allowed for the electron in the atom, then it must have only certain E values, and not others.

In other words:

Line spectrum → Quantized energy levels

Quantized energy levels

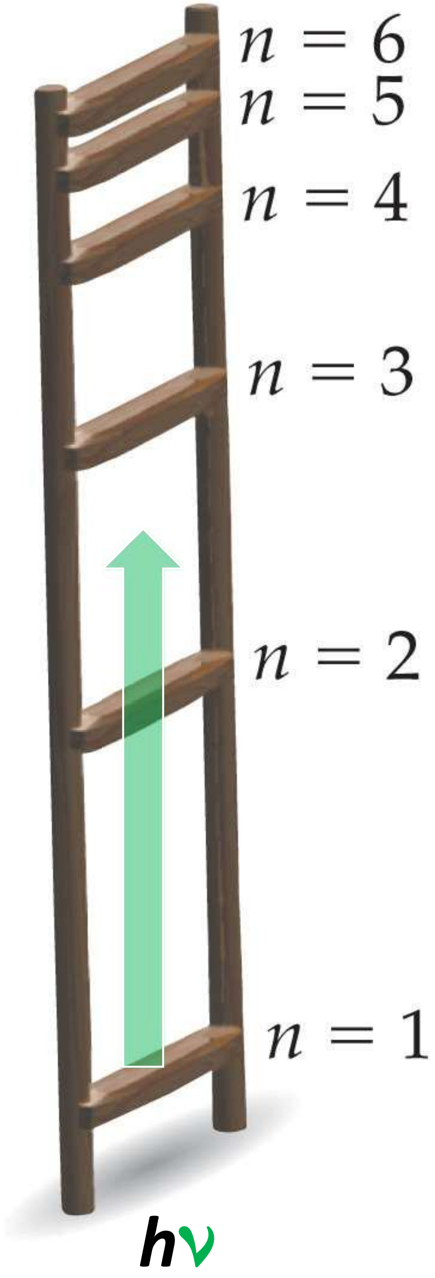
Just as we can only step on the individual levels on a ladder, the electrons in an atom can only exist at certain energy levels and not in between.



Quantized energy levels

If the energy of the photon doesn't match an energy difference between two levels in an atom, it's not absorbed.

Even if it has more than enough energy!

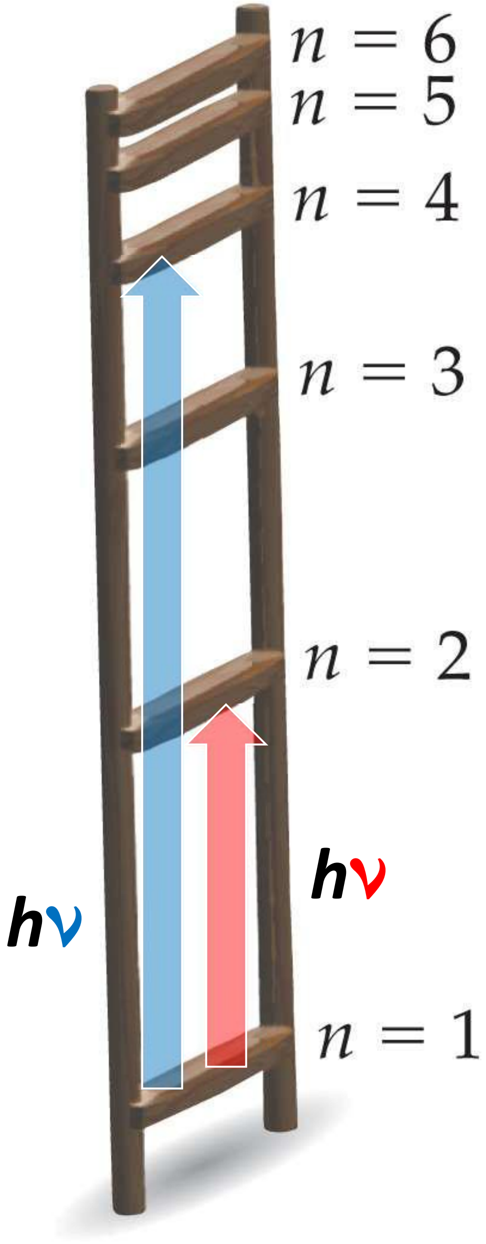


Quantized energy levels

If the energy of the photon matches a difference between two levels exactly, it can be absorbed.

Not more, not less, exactly the same.

$$\underset{\substack{\uparrow \\ h\nu}}{E_{\text{photon}}} = \Delta E_{\text{electron}}$$



But why are energy levels in atoms quantized?

Particles as waves

Before we go further, we need to appreciate the wave nature of matter a bit more.

De Broglie's leap of faith:

Take Planck's $E_{photon} = h\nu = \dfrac{hc}{\lambda}$ (applies to photons)

Combine it with Einstein's $E = mc^2$ (applies to everything)

$$\Rightarrow \quad m = \frac{E}{c^2} = \frac{hc/\lambda}{c^2} = \frac{h}{\lambda c}$$

$$\begin{tikzcd} \Rightarrow \quad \lambda = \dfrac{h}{m\,c} \arrow[d, bend left, "?"] & \boxed{\text{for photons}} \\ \lambda = \dfrac{h}{m\,v} & \boxed{\text{for all particles}} \end{tikzcd}$$

See if it applies to everything.

It does!

Wavelength of a particle!

$$\boxed{\lambda = \frac{h}{mv}}$$

De Broglie equation

Practice:
Check your solution on next page

- Calculate the wavelength of an electron traveling at 2.65×10^6 m/s

m of an e^- = 9.11×10^{-31}kg

h=6.626×10^{-34}J.s (J=kgm^2/s)

Practice: Calculate the wavelength of an electron traveling at 2.65 x 10^6 m/s

Given: v = 2.65 x 10^6 m/s, m = 9.11 x 10^{-31} kg (back leaf)

Find: λ, m

Conceptual Plan:

$$m, v \xrightarrow{\qquad} \lambda\ (m)$$

$$\lambda = \frac{h}{m \bullet v}$$

Relationships: λ=h/mv

Solve:

$$\lambda = \frac{h}{mv} = \frac{\left(6.626 \times 10^{-34}\ \frac{\cancel{kg} \bullet \cancel{m}^2}{\cancel{s}^2} \bullet \cancel{s}\right)}{\left(9.11 \times 10^{-31}\ \cancel{kg}\right)\left(2.65 \times 10^{6}\ \frac{\cancel{m}}{\cancel{s}}\right)}$$

$$= 2.74 \times 10^{-10}\ m$$

Particles as waves

- A stable state for a wave in a confined space is a "standing wave"
  - Like the vibrations of a guitar string

- So when we confine a particle into a limited space, the standing wave requirement allows only certain wavelengths and excludes all others

“Particle in a box”

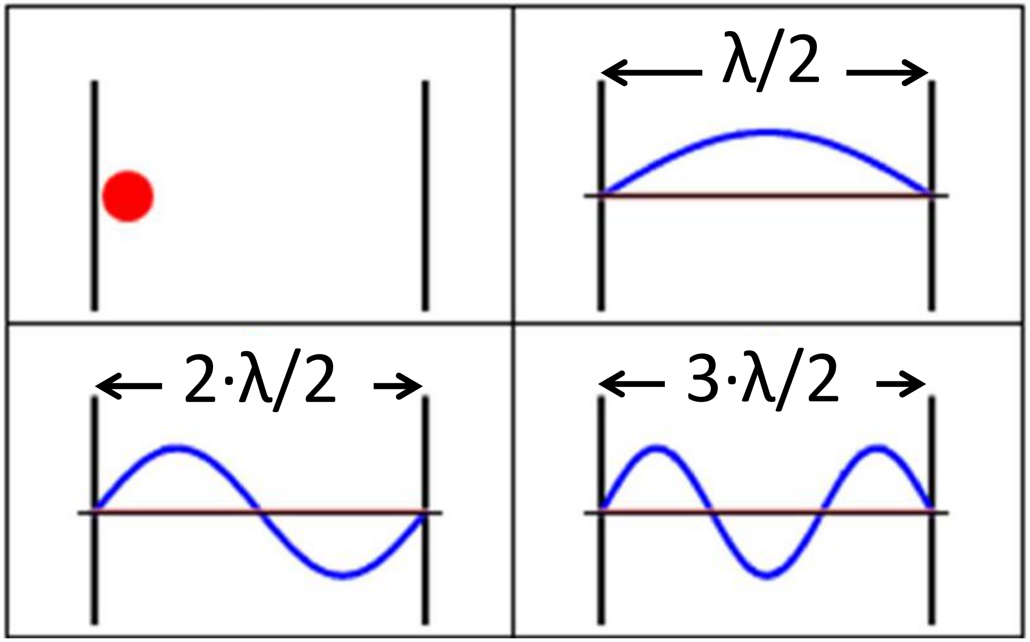
A particle is a wave with a de Broglie wavelength of λ

It can only fit in a “box” if the box’s length is a multiple of λ/2

So only certain λ values are allowed

Therefore only certain particle speeds are allowed.

Therefore only certain particle energies are allowed.

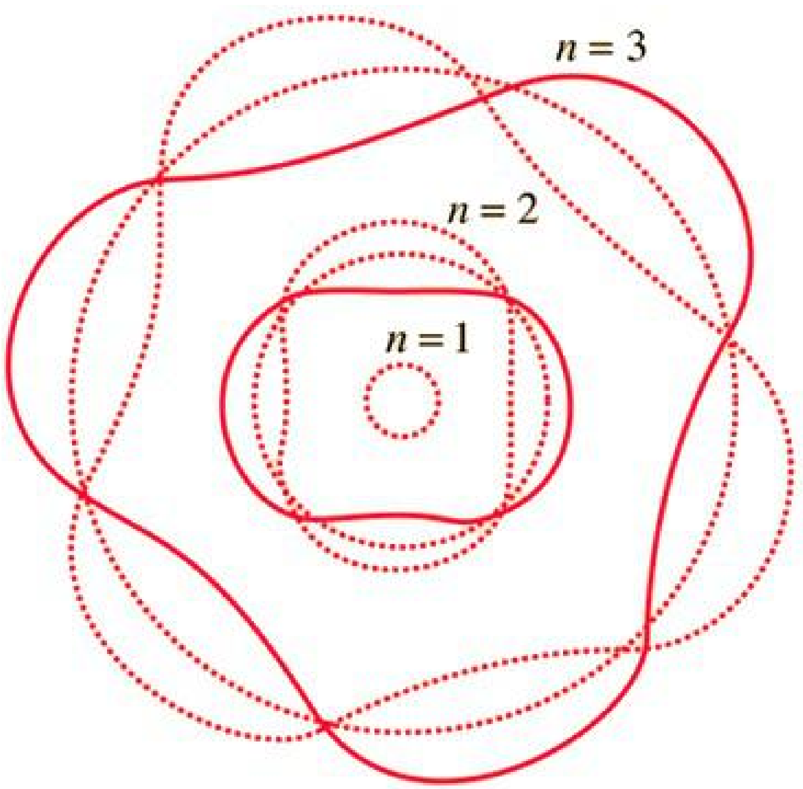


If the box is infinitely big
then λ isn’t restricted

© Arno Papazyan

en.wikipedia.org/wiki/Particle_in_a_box

- An electron constrained to be around the nucleus (because of the electrostatic attraction to the nucleus) is also in a kind of circular "box".
- The circle length still needs to be a multiple of λ/2



Bohr Model of the Hydrogen Atom

- Before de Broglie derived his result, Bohr came up with a model for Hydrogen atom.
  - ➢ But it was (later) explainable by the de Broglie wavelength

- Electrons “orbit” around the nucleus, the (+)/(-) attractions balanced by the centrifugal forces

- A simple but unexplained assumption is made about the allowed angular speeds of the electrons. And ta-da!

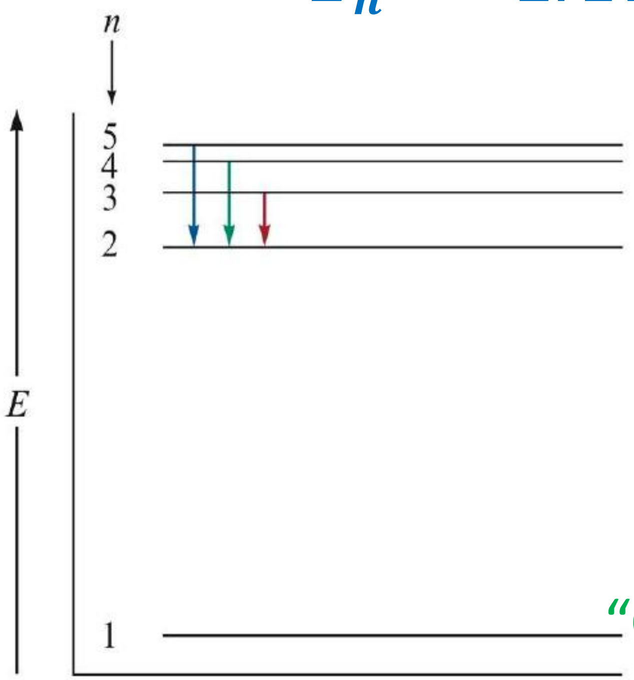
Bohr’s model gave hydrogen atom energy levels consistent with the hydrogen emission spectrum.

Bohr Model of the Hydrogen Atom

- It gives a “caricature” picture of a hydrogen atom
- Electrons can be imagined to “jump” between orbits, which correspond to different energy levels.
- An electron can jump up between levels when supplied with just the right amount of energy between two levels
- When an electron jumps down between levels, the energy is lost in the form of an emitted photon.

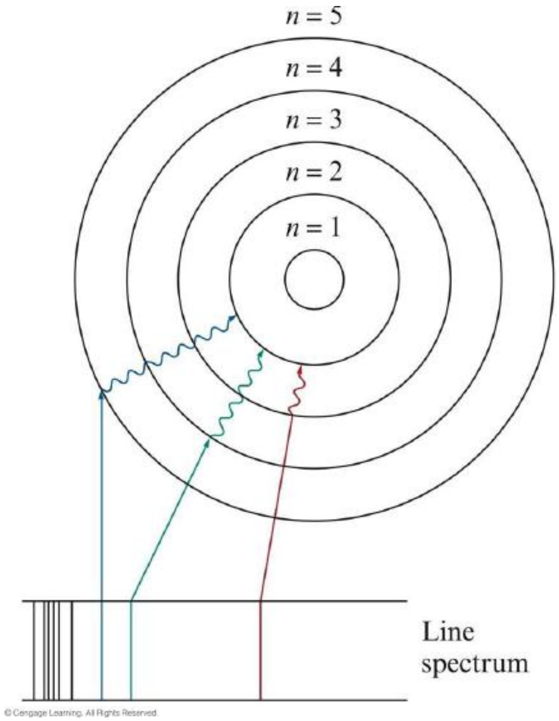
Energy levels & electronic transitions in the Bohr model

$$E_n = -2.178 \times 10^{-18}\text{J}\ \frac{1}{n^2}$$



“Excited states”

“Ground state”



Change in energy of the atom:

$$\Delta E = -2.178 \times 10^{-18}\text{J} \left(\frac{1}{n^2_{final}} - \frac{1}{n^2_{\text{initial}}} \right)$$

Energy levels and "transitions" for the electron in an atom

- Ground state – lowest possible energy state (n = 1)
- Electrons can be "excited" to higher levels (n=2, 3, 4, …) by absorbing a photon with an energy that equals the energy difference between levels

E_{photon} is always positive

$$E_{\text{photon}} = |\Delta E_{\text{transition}}|$$

Bohr Model of the Hydrogen Atom

For any electronic transition, we have:

$$|\Delta E_{transition}| = E_{photon} = h\nu = \frac{hc}{\lambda}$$

Frequency and wavelength of light corresponding to the transition are given by the energy change in the transition

Example

Calculate the wavelength of light emitted when an excited electron in the hydrogen atom falls from n = 5 to n = 2

The energy of the transition is given by: $\Delta E = -2.178 \times 10^{-1}\ \mathrm{J}\left(\frac{1}{n^2_{final}} - \frac{1}{n^2_{\mathrm{initial}}}\right)$

whose magnitude gives the photon energy: $|\Delta E_{transition}| = E_{photon} = h\nu = \frac{hc}{\lambda}$

then λ is given by: $\lambda = hc/\ E_{photon}$

Applying these thoughts:

$$\Delta E = -2.178 \times 10^{-1}\ \mathrm{J}\left(\frac{1}{2^2} - \frac{1}{5^2}\right) = -4.574\mathrm{x}10^{-19}\ \mathrm{J}$$

$$E_{photon} = |-4.574\mathrm{x}10-19\ \mathrm{J}\ | = 4.574\mathrm{x}10^{-19}\ \mathrm{J}$$

$$\lambda = (6.626\mathrm{x}10^{-34}\ \mathrm{J{\cdot}s})(3.00\mathrm{x}10^{-8}\ \mathrm{m/s})\ /\ (4.574\mathrm{x}10^{-19}\ \mathrm{J}) = 4.34\mathrm{x}10^{-7}\ \mathrm{m}$$

$$\lambda = (4.34\mathrm{x}10^{-7}\ \mathrm{m})(1\ \mathrm{nm}\ /\ 10^{-9}\ \mathrm{m}) = 434\ \mathrm{nm}$$

Practice (Check your solution on next page)

Calculate the wavelength of light emitted when the hydrogen electron transitions from $n = 2$ to $n = 1$

Practice (Check your solution on next page)

Calculate the wavelength of light emitted when the hydrogen electron transitions from $n = 2$ to $n = 1$

Given: $n_i = 2,\ n_f = 1$

Find: λ, m

Conceptual Plan:

$$n_i,\ n_f \xrightarrow{\;E = -R_H\left(\frac{1}{n^2}\right)\;} \Delta E_{atom} \xrightarrow{\;\Delta E_{atom} = -E_{photon}\;} E_{photon} \xrightarrow{\;\lambda = \frac{h \bullet c}{E}\;} \lambda$$

Relationships: $E = hc/\lambda$, $E_n = -2.18 \times 10^{-18}\ \text{J}\ (1/n^2)$

Solve:

$$\Delta E_{atom} = -2.18 \times 10^{-18}\ \text{J}\left(\frac{1}{1^2} - \frac{1}{2^2}\right) = -1.64 \times 10^{-18}\ \text{J}$$

$$E_{photon} = -(-1.64 \times 10^{-18}\ \text{J}) = 1.64 \times 10^{-18}\ \text{J}$$

$$\lambda = \frac{hc}{E} = \frac{\left(6.626 \times 10^{-34}\ \text{J} \bullet \text{s}\right)\left(3.00 \times 10^{8}\ \frac{\text{m}}{\text{s}}\right)}{\left(1.64 \times 10^{-18}\ \text{J}\right)} = 1.21 \times 10^{-7}\ \text{m}$$

Check: the unit is correct, the wavelength is in the UV, which is appropriate because it is more energy than 3→2 (in the visible)

Practice:
Check your solution on next page

A photon with an energy of **4.42×10^{-19} J** is able to free an electron from the surface of Cesium metal and give it the leftover energy in the form of kinetic energy. Could that photon excite an electron in a hydrogen atom from n=2 to n=3?

Practice

A photon with an energy of **4.42x10^{-19} J** is able to free an electron from the surface of Cesium metal and give it the leftover energy in the form of kinetic energy. Could that photon excite an electron in a hydrogen atom from n=2 to n=3?

Energy change in electronic transitions in a hydrogen atom is given by:

$$\Delta E = -2.178 \times 10^{-18}\text{J}\left(\frac{1}{n_{final}^2} - \frac{1}{n_{\text{initial}}^2}\right)$$

$$\Delta E = -2.178 \times 10^{-18}\text{J}\left(\frac{1}{3^2} - \frac{1}{2^2}\right) \quad \mathbf{= 3.025x10^{-19}\ J}$$

$$4.42\text{x}10^{-19}\ \text{J} \ > \ 3.025\text{x}10^{-19}\ \text{J}$$

The photon has more energy than required to make the electron jump from n=2 to n=3.

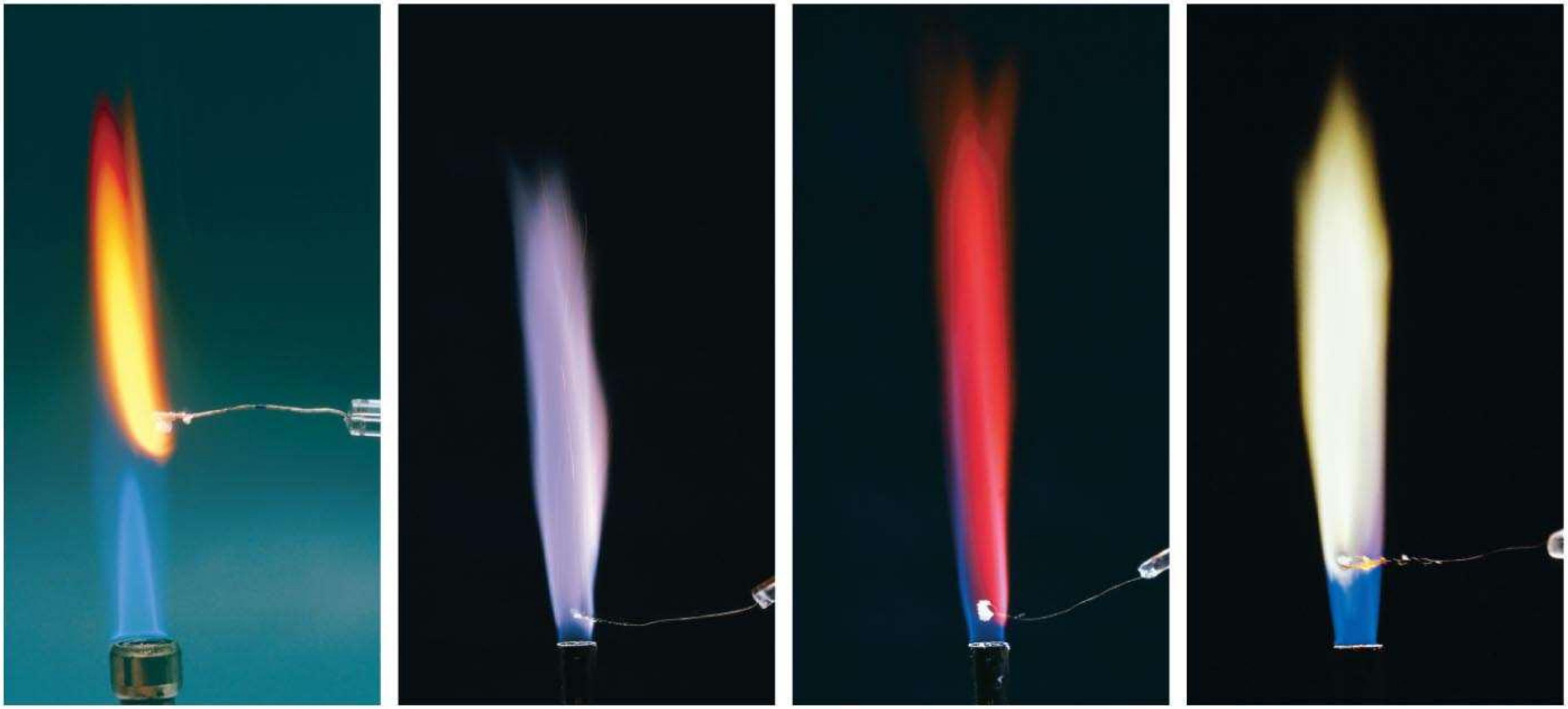
But its energy doesn't match the transition energy!
It cannot excite the electron even if it has more than enough energy!

Spectra

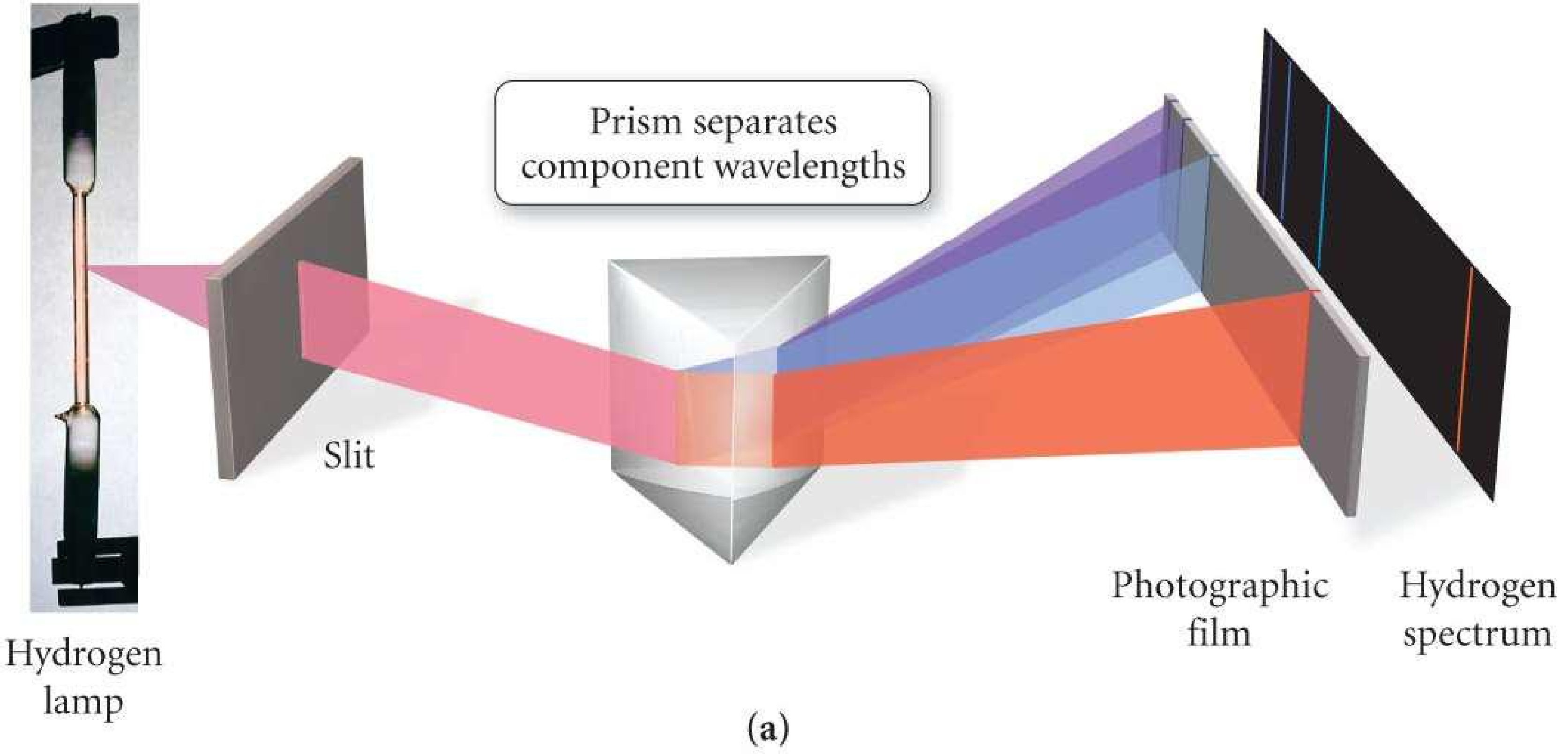
- When atoms or molecules absorb energy, that energy is often released as light energy
  - fireworks, neon lights, etc.
- When that emitted light is passed through a prism, a pattern of particular wavelengths of light is seen that is unique to that type of atom or molecule – the pattern is called an **emission spectrum**
  - non-continuous
  - can be used to identify the material
    - flame tests

Exciting Gas Atoms to Emit Light with Electrical Energy

Identifying Elements with Flame Tests

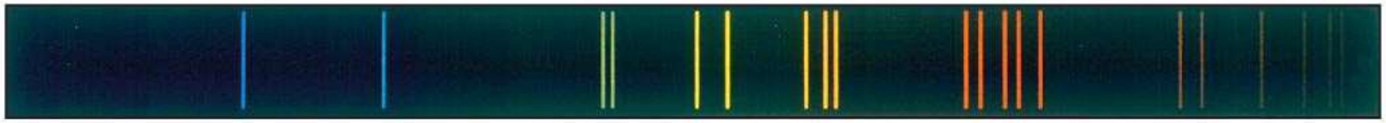


Emission Spectra



Examples of Spectra

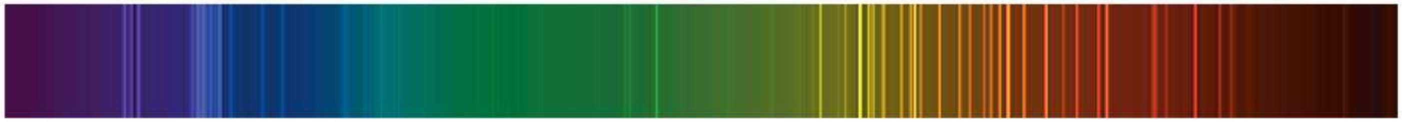
Helium spectrum



Barium spectrum

White light spectrum

Oxygen



Neon

Bohr model & formula fails for atoms with more than one electron!

- Bohr model doesn’t really capture the fundamental reason for the discrete, “quantized” energy levels
- It failed to predict the energy levels and the transition energies for other elements
  - When there is more than one electron
- A true explanation was provided by Quantum Mechanics, based on the wave nature of electrons.

The Quantum-Mechanical Model: Atoms with Orbitals

- Quantum mechanics revolutionized physics and chemistry because, in the quantum-mechanical model, electrons *do not* behave like particles flying through space.
- We cannot, in general, describe their exact paths.

Quantum Mechanics gives us probabilities

- Quantum mechanics only tells us probabilities, not the exact location of particles.
- "Solving" the quantum mechanical equation for an atom gives us 3-dimensional functions that describe where the electron is most likely to be found, and the energy corresponding to that particular solution
- The result is a cloud-like description of "probability density", which is in effect "electron density" around a nucleus
- Each possible function ("**wavefunction**") is called an "**orbital**" (**not** "orbit" as Bohr's model assumed)

Quantum Mechanics of the Atom

Each distinct solution to the H atom wavefunction is called an “**orbital**”

An orbital defines where in space an electron is likely to be found.

In other words:

- The electron is smeared into a “fog”, and an orbital describes where that fog is dense.
- The region where electron density is high describes the shape and size of an orbital

Orbital Size

- Difficult to define precisely.

Lowest energy Hydrogen orbital is a spherical cloud

Radius of the sphere that encloses 90% (or 99%, or whatever; it doesn’t change what it looks like) of the total electron probability.

Lowest energy orbital for Hydrogen

Just one of many solutions for the electron wavefunction in Hydrogen

intensity of color denotes here the probability density at any given point

A set of "Quantum numbers" define an orbital

Consider a simple, one-dimensional function like

$y = ax^b + cx$

It has a general form, but it's not totally specified until we specify the factors a, b, c.

- Similarly, there are "Quantum numbers" that specify the exact form of the 3-dimensional orbital function. Their allowed values are determined when the quantum mechanical equation is solved.

A set of “Quantum numbers” define the “address” of an electron

The quantum numbers form a hierarchy

The “principal” quantum number defines a “**shell**”

Within each shell there are “**subshells**”

Within each subshell there are **orbitals**

Each orbital can contain up to two **electrons**

A set of “Quantum numbers” define the “address” of an electron

Now thinking in the opposite direction,

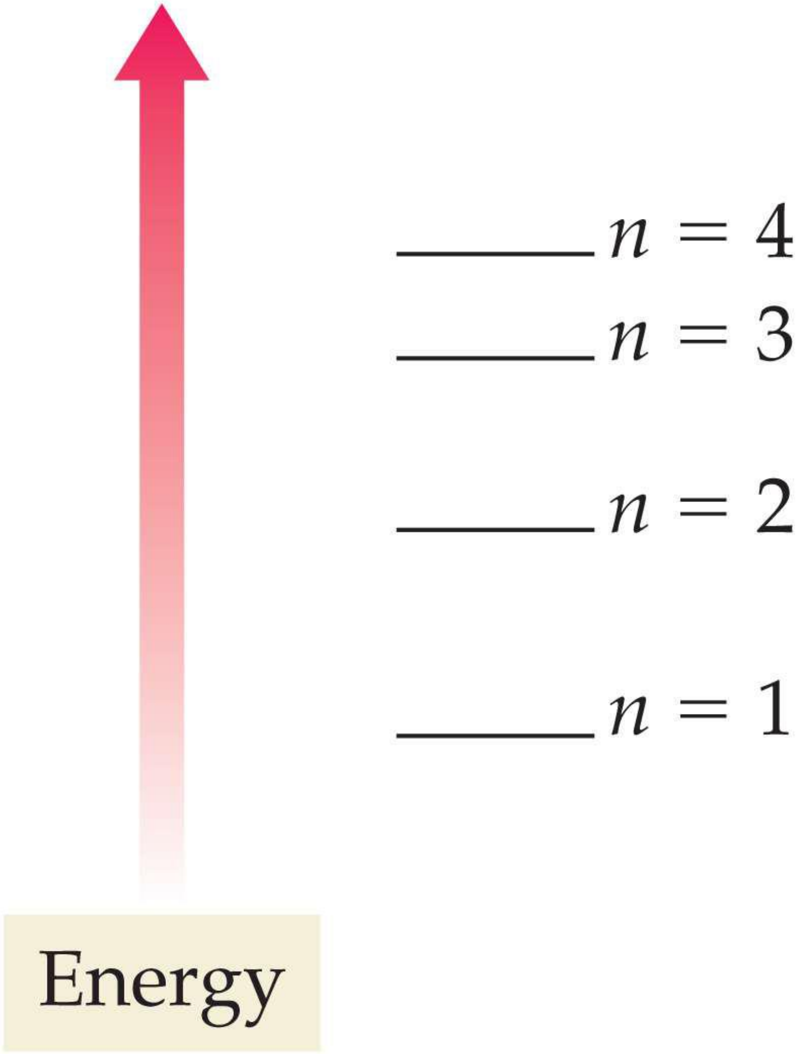
- An electron in an atom can be alone in an orbital, or share it with another electron.
- That orbital is in a subshell
- That subshell is in a shell

The Quantum-Mechanical Model: Atoms with Orbitals

We will explicitly use numbers only for “shell number”

Energy Increases with Principal Quantum Number

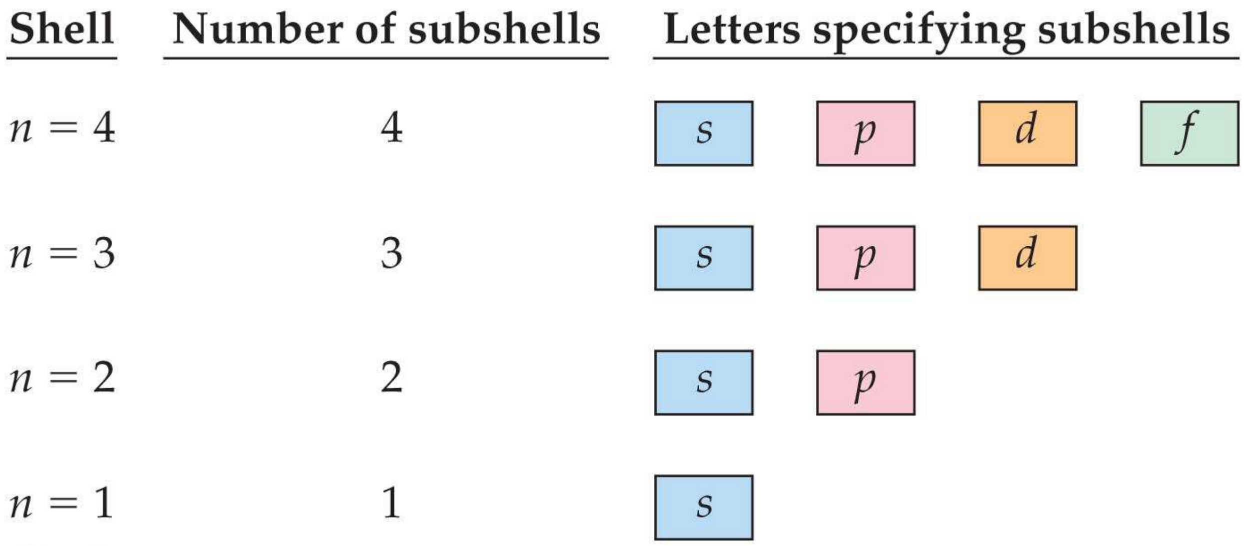
- The higher the principal quantum number, the higher the energy of the orbital.
- The possible principal quantum numbers are
  n = 1, 2, 3 …
- Energy increases with n
- Distance from nucleus also increases with n



The Number of Subshells in a Given Principal Shell Is Equal to the Value of *n*

Each shell is composed of subshells

Conveniently, number of subshells in a shell is equal to the "shell number" (principal quantum number)

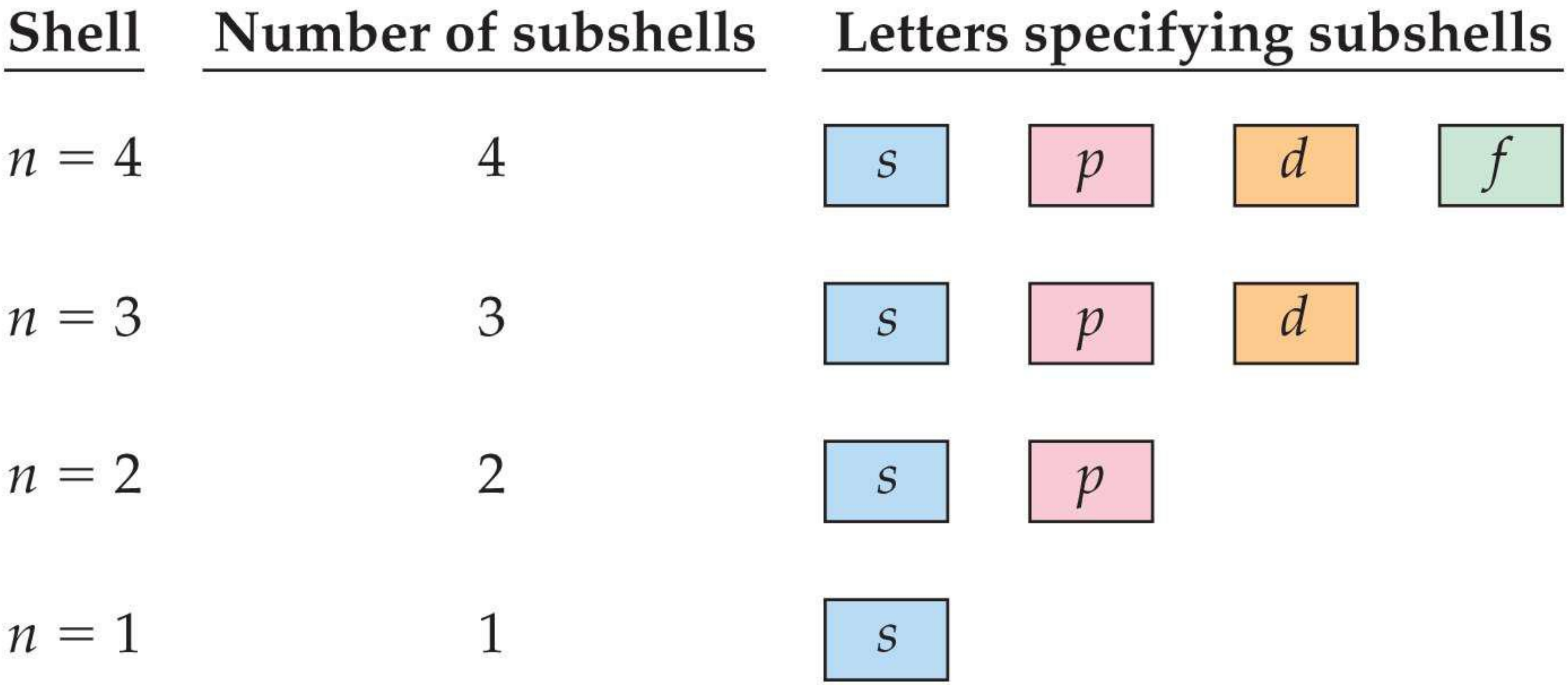


Shell	Number of subshells	Letters specifying subshells			
$n = 4$	4	*s*	*p*	*d*	*f*
$n = 3$	3	*s*	*p*	*d*	
$n = 2$	2	*s*	*p*		
$n = 1$	1	*s*			

Subshells are usually represented by letters (we won’t use the actual number)

Subshell determines the shape of the orbitals within it

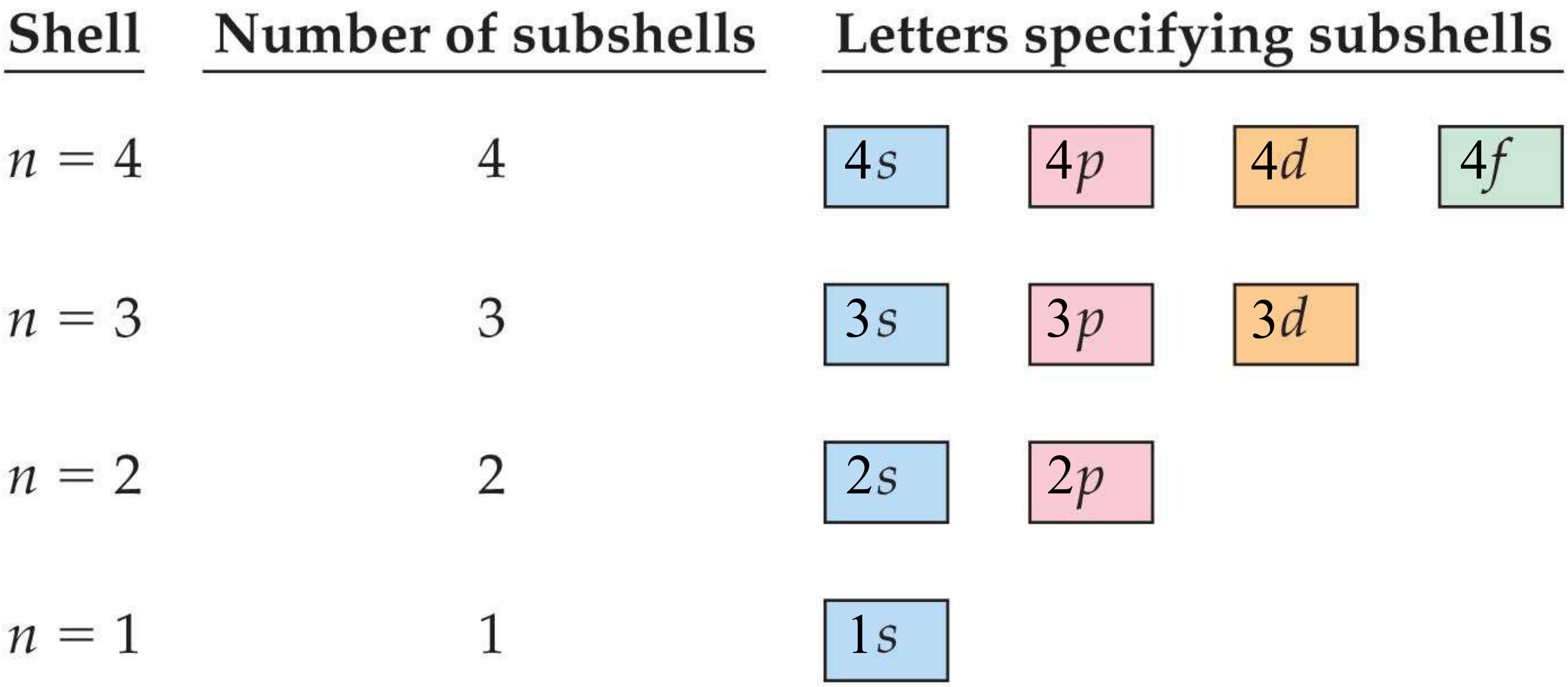
Each subshell has a letter designation



Shell	Number of subshells	Letters specifying subshells			
$n = 4$	4	*s*	*p*	*d*	*f*
$n = 3$	3	*s*	*p*	*d*	
$n = 2$	2	*s*	*p*		
$n = 1$	1	*s*			

Within each shell, the same letters *s, p, d, f,* etc. are used to designate subshells

The full designation for a subshell includes the shell number



Shell	Number of subshells	Letters specifying subshells			
$n = 4$	4	$4s$	$4p$	$4d$	$4f$
$n = 3$	3	$3s$	$3p$	$3d$	
$n = 2$	2	$2s$	$2p$		
$n = 1$	1	$1s$			

Number of orbitals in a subshell: depends only on its letter designation

Shell	Number of subshells	Letters specifying subshells			
$n = 4$	4	$4s$	$4p$	$4d$	$4f$
$n = 3$	3	$3s$	$3p$	$3d$	
$n = 2$	2	$2s$	$2p$		
$n = 1$	1	$1s$			

Number of orbitals in any ***s***-subshell = **1**

Number of orbitals in any ***p***-subshell = **3**

Number of orbitals in any ***d***-subshell = **5**

Number of orbitals in any ***f***-subshell = **7**

Orbitals in a given subshell carry the same letter designation as the subshell

- with a subscript label to distinguish them if needed

Representations of Orbitals

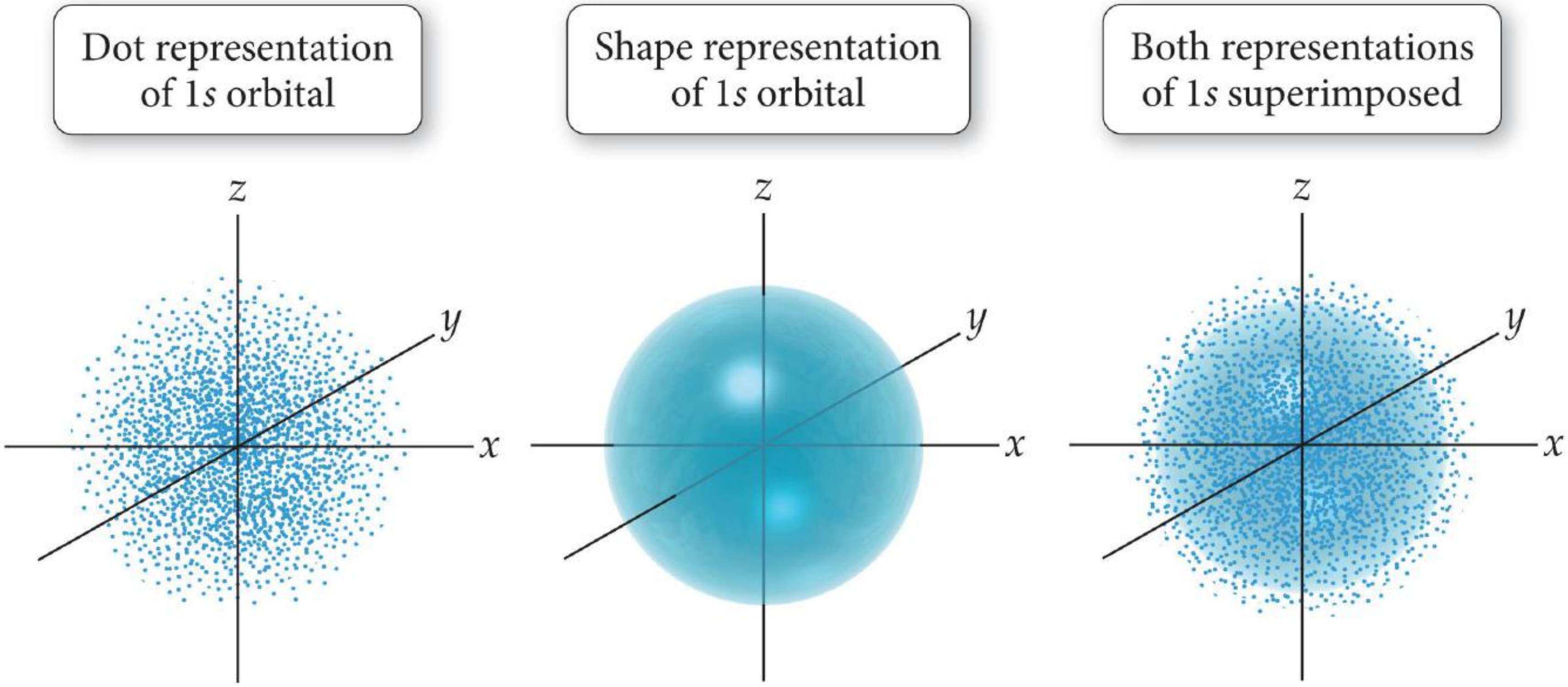
- Orbitals are sometimes represented by a cloud of dots, where the dot density is proportional to the probability of finding the electron.
- The ***dot density*** for the 1*s* orbital is greatest near the nucleus and decreases farther away from the nucleus.
- The electron is more likely to be found close to the nucleus than far away from it.

Representations of Orbitals

- Orbitals can be represented as ***geometric shapes*** that encompass most of the volume where the electron is likely to be found.
- The 1*s* orbital can be represented as a sphere that encompasses the volume within which the electron is found 90% of the time.
- If we superimpose the dot representation of the 1*s* orbital on the shape representation, we can see that most of the dots are within the sphere, meaning that the electron is most likely to be found within the sphere when it is in the 1*s* orbital.

Representations of Orbitals

- The dot density is proportional to the probability of finding the electron.
- The greater dot density near the middle represents a higher probability of finding the electron near the nucleus.

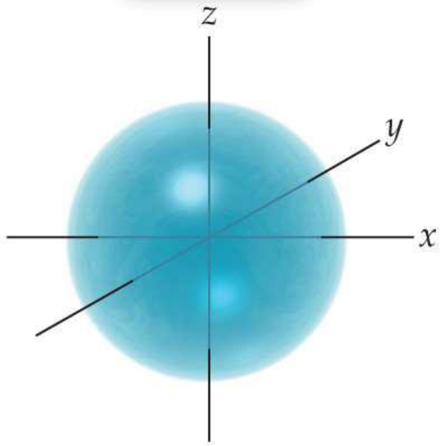

Dot representation of 1*s* orbital

Shape representation of 1*s* orbital

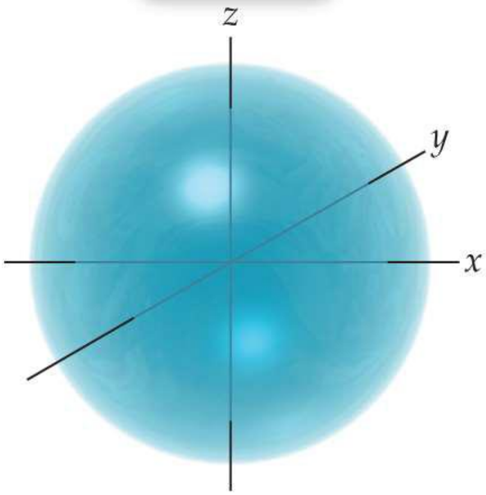
Both representations of 1*s* superimposed

The 2*s* Orbital Is Similar to the 1*s* Orbital, but Larger in Size

1*s* orbital



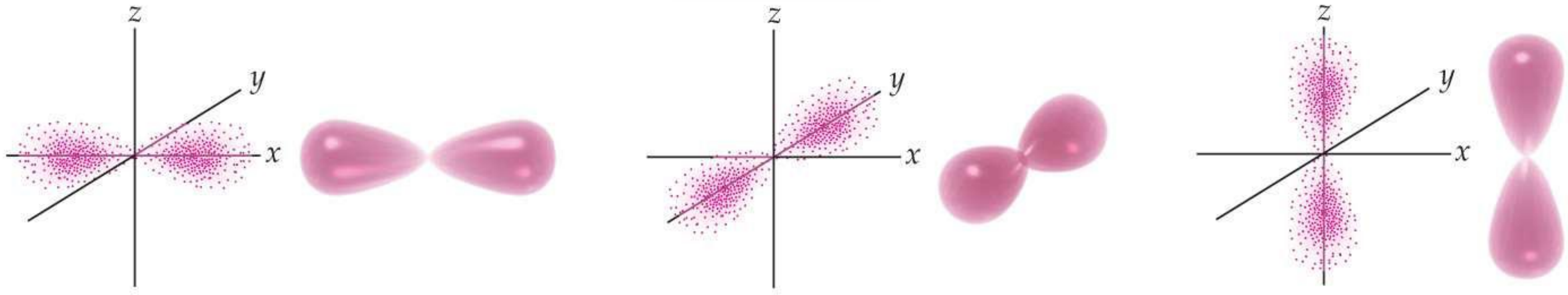
2*s* orbital



The 2*p* Orbitals: The orbitals in the 2*p* subshell (When *n*=2 and the subshell letter is *p)*

Dot representation (Left) and shape representation (Right) for each *p* orbital:

The 2*p* orbitals



(a) p_x (b) p_y (c) p_z

p-orbitals are “dumbbell shaped”

Orbitals When *n* = 3

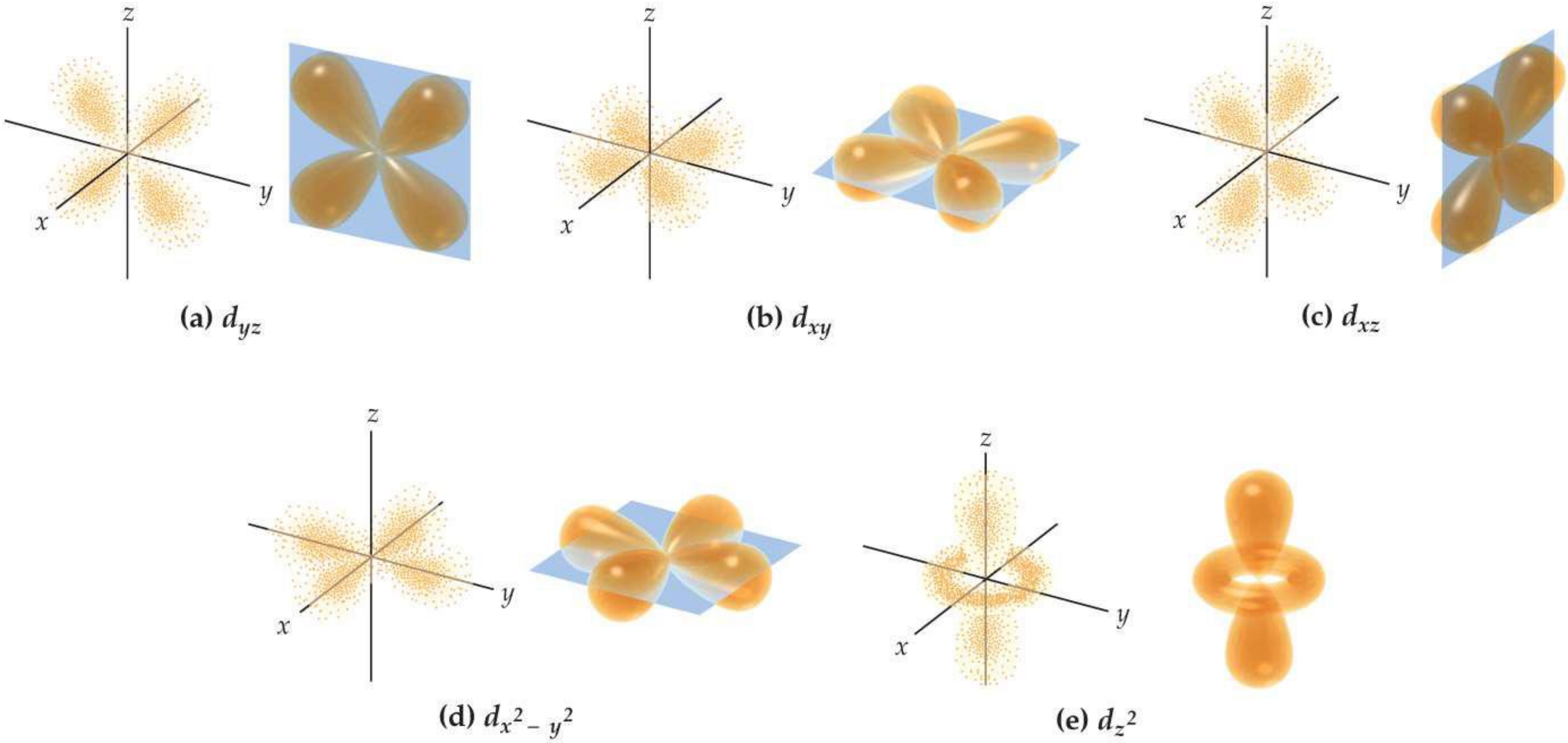
- The next principal shell, *n* = 3, contains three subshells specified by *s*, *p*, and *d:*

  3*s*, 3*p*, and 3*d*

- Orbitals in 3*s* and 3*p* subshells are similar in shape to the 2*s* and 2*p* orbitals, but slightly larger and higher in energy.
- Again, one orbital in 3*s*, and three orbitals in 3*p*
- The *d* subshell contains five *d* orbitals.

The 3*d* Orbitals: Orbitals in the 3*d* subshell The Dot (Left) and Shape (Right) representations for Each *d* Orbital

The 3*d* orbitals



(a) d_{yz} (b) d_{xy} (c) d_{xz}

(d) $d_{x^2-y^2}$ (e) d_{z^2}

Why are Atoms Spherical?

Orbital Diagrams

- Instead of showing actual pictures of the electron clouds, we summarize the "addresses" of electrons in an atom as an "electron configuration".
- One way to do that is an **orbital diagram:** the electrons as arrows, in a box representing the orbital.
- The orbital diagram for a ground-state hydrogen atom is as follows:

Why an arrow?

Because an electron acts like a spinning charge, making it a tiny magnet. Let's say:

Clockwise spin is magnet pointing up

Counterclockwise spin is magnet pointing down

Electron Spin

- In orbital diagrams, the direction of the arrow (pointing up or pointing down) represents the direction of its magnet, known as **electron spin**
- The **Pauli exclusion principle:**
  - **No two electrons can be in the same specific orbital and also have the same spin,** which means:
- *An orbital may hold no more than two electrons, and those electrons must have opposite spins*.
- Two electrons with opposite spins are represented as

A consequence of the Pauli Exclusion Principle:

The “Pauli Exclusion Principle imposes a capacity of two electrons per orbital.

This forces electrons to populate higher energy subshells as they fill and run out of unfilled orbitals in a subshell.

We now turn our attention to the energy order of those subshells …

Using the concepts of shell, subshell, orbital for all elements

All the quantum numbers, shells, subshells, orbitals we have seen are derived for the Hydrogen atom:

1 electron

They technically apply only to Hydrogen

But it turns out:

- We can apply the concepts (shells, subshells, orbitals) developed for H atom to other atoms,
- But there are “complications”

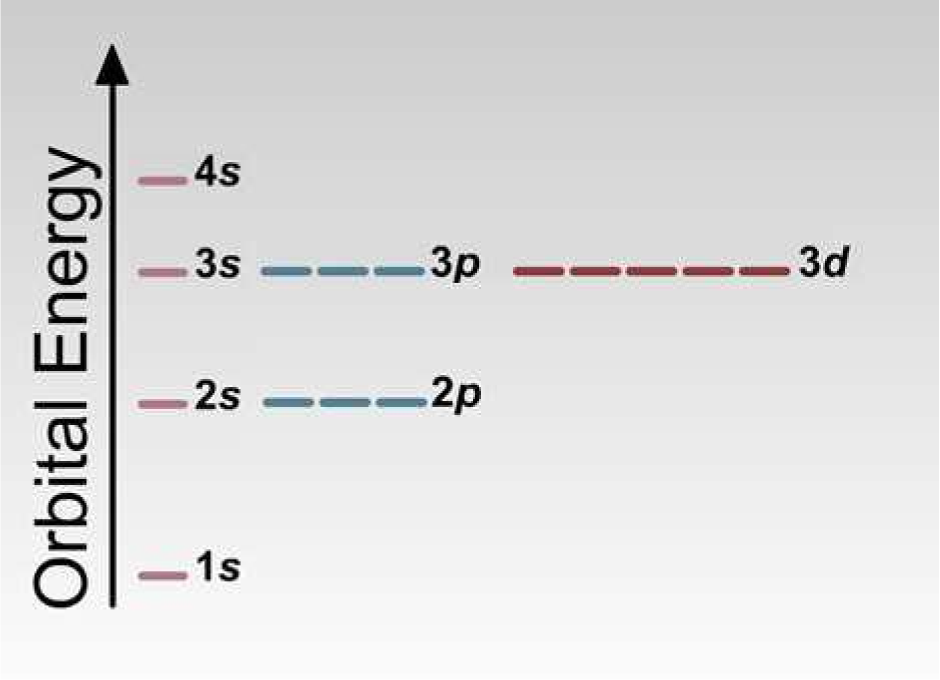
For Hydrogen there is only one electron around the nucleus, and all subshells in a given shell have the same energy.

For atoms with more than one electron:

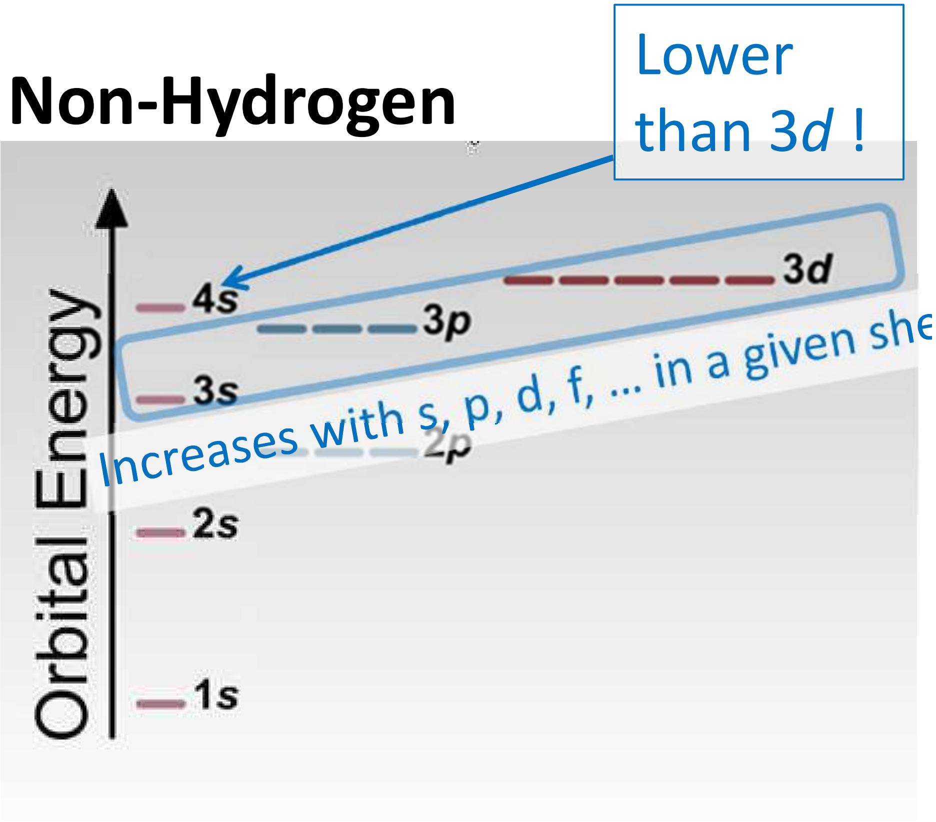
- Electron-electron repulsions affect subshell energies
- In a given shell, energy of subshells increase with the order *s*, *p*, *d*, *f*, …
- *But the s-subshell of the next shell always turns out to be lower than the d-subshell of the given shell! (relevant after n=3)*

Subshell energies

Hydrogen



Non-Hydrogen



In non-hydrogen atoms:

- Subshells in a shell are not of equal energy
- A subshell in a higher shell might have a lower energy than one in a lower shell

Aufbau (build-up) Principle

Electrons in an atom are “built up” by adding them into the available orbitals in subshells in the order of increasing energy.

A lower energy subshell is filled first, followed by higher energy subshells.

This leads to “**ground-state**” electron configurations.

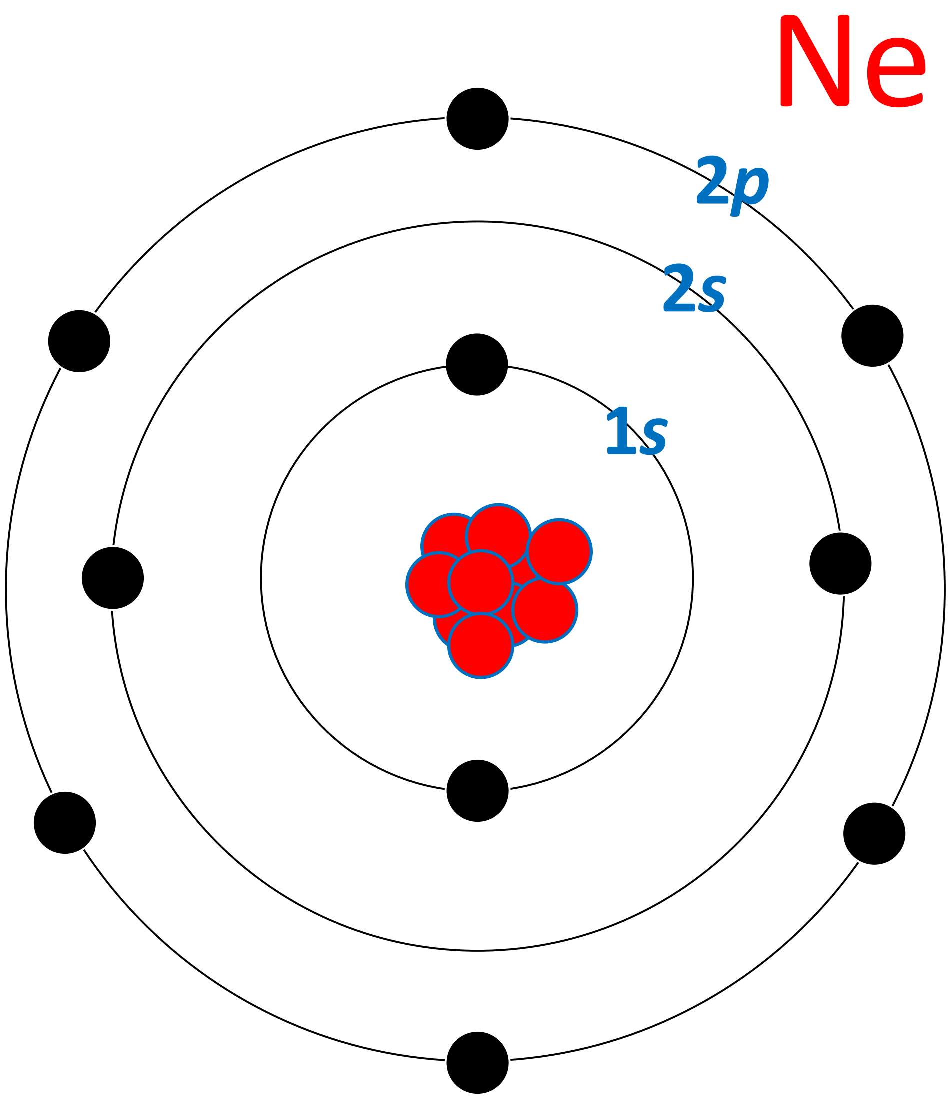
To build-up the next element, and then the next ….

- For each proton added to the nucleus:

  --- Electrons are added to hydrogen-like orbitals (which are in subshells designated by *s, p, d, f*, …).

“Building up” atoms

For each proton we add to the nucleus to make the next atom, we add an electron into the lowest unfilled subshell



- The neutrons needed to keep the protons together are not shown
- Relative size of the nucleus is much, much smaller than shown
- Electrons are actually **<u>not</u>** “dots” on a fixed orbit

Electron Configurations

The format of the electron configuration is:

$\{\text{shell number}\}\{\textit{subshell letter}\}^{\text{number of electrons}}$

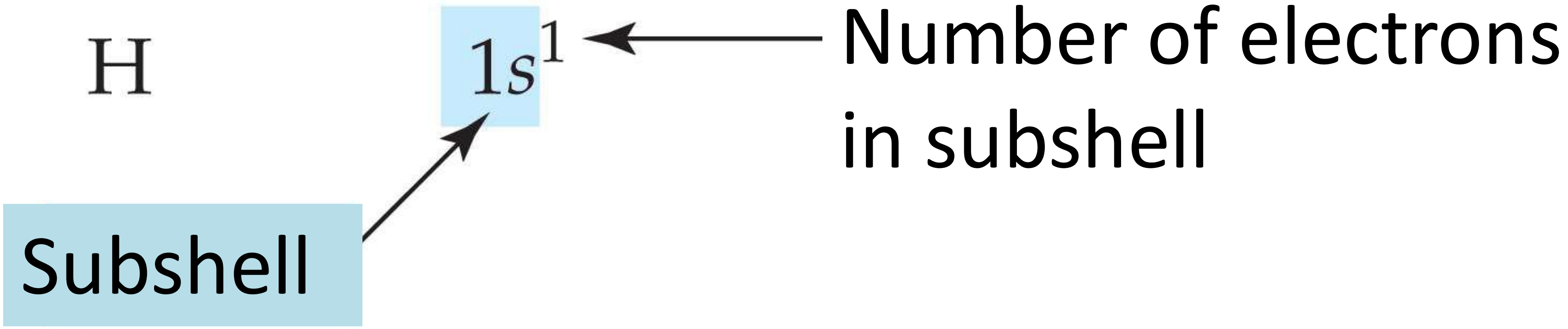
repeated for each subshell, in the order
nature populates them,
i.e. in the order of increasing energy

For now, we'll start with electron configurations of lighter elements

- where the order of orbital energies don't yet get complicated
- up to Argon, at the end of the 3rd period of the periodic table

Electron Configurations

- An **electron configuration** shows the occupation of subshells by electrons for a particular atom.
- The electron configuration for a ground-state hydrogen atom is as follows:



H $1s^1$

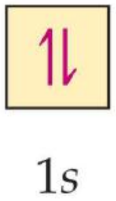
Number of electrons in subshell

Subshell

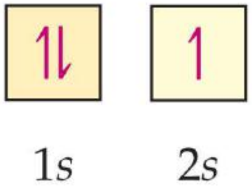
- The electron configuration tells us that hydrogen’s single electron is in the 1*s* subshell (which is also the sole 1*s* orbital.)

Writing Ground-State Electron Configurations

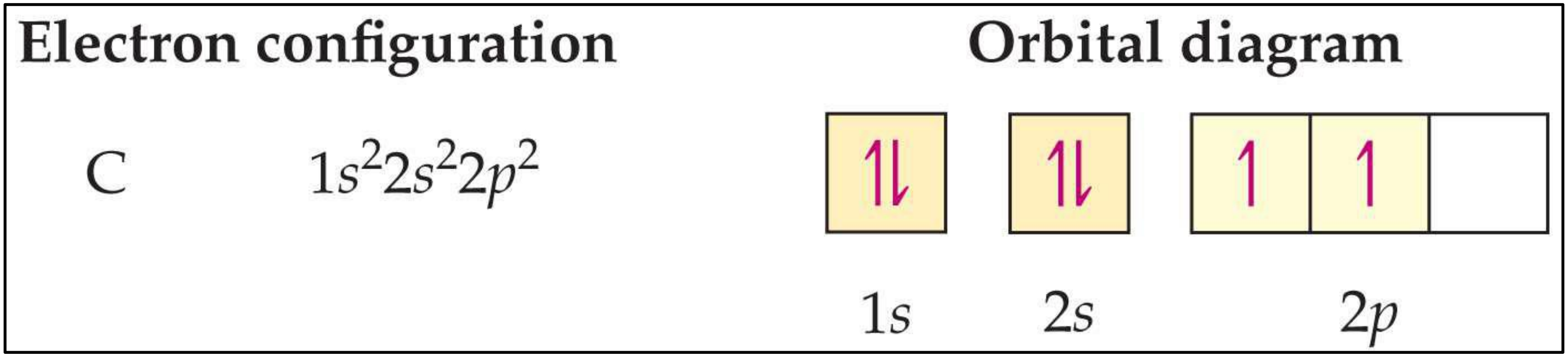
- A **helium** atom has two electrons.
- The electron configuration and orbital diagram for helium are as follows:

	Electron configuration	Orbital diagram
He	$1s^2$	

- A **lithium** atom has three electrons.
- The electron configuration and orbital diagram for lithium are as follows:

	Electron configuration	Orbital diagram
Li	$1s^22s^1$	

For carbon, which has six electrons, the electron configuration and orbital diagram are as follows:



- The 2*p* electrons occupy the *p* orbitals (of equal energy) ***singly***, rather than pairing in one orbital.

This is the result of **Hund's rule:**

- *When filling orbitals of equal energy, electrons fill them singly first, with parallel spins.*

Writing Ground-State Electron Configurations

Hund’s rule:

- *When filling orbitals of equal energy, electrons fill them singly first, with parallel spins.*

To recap:

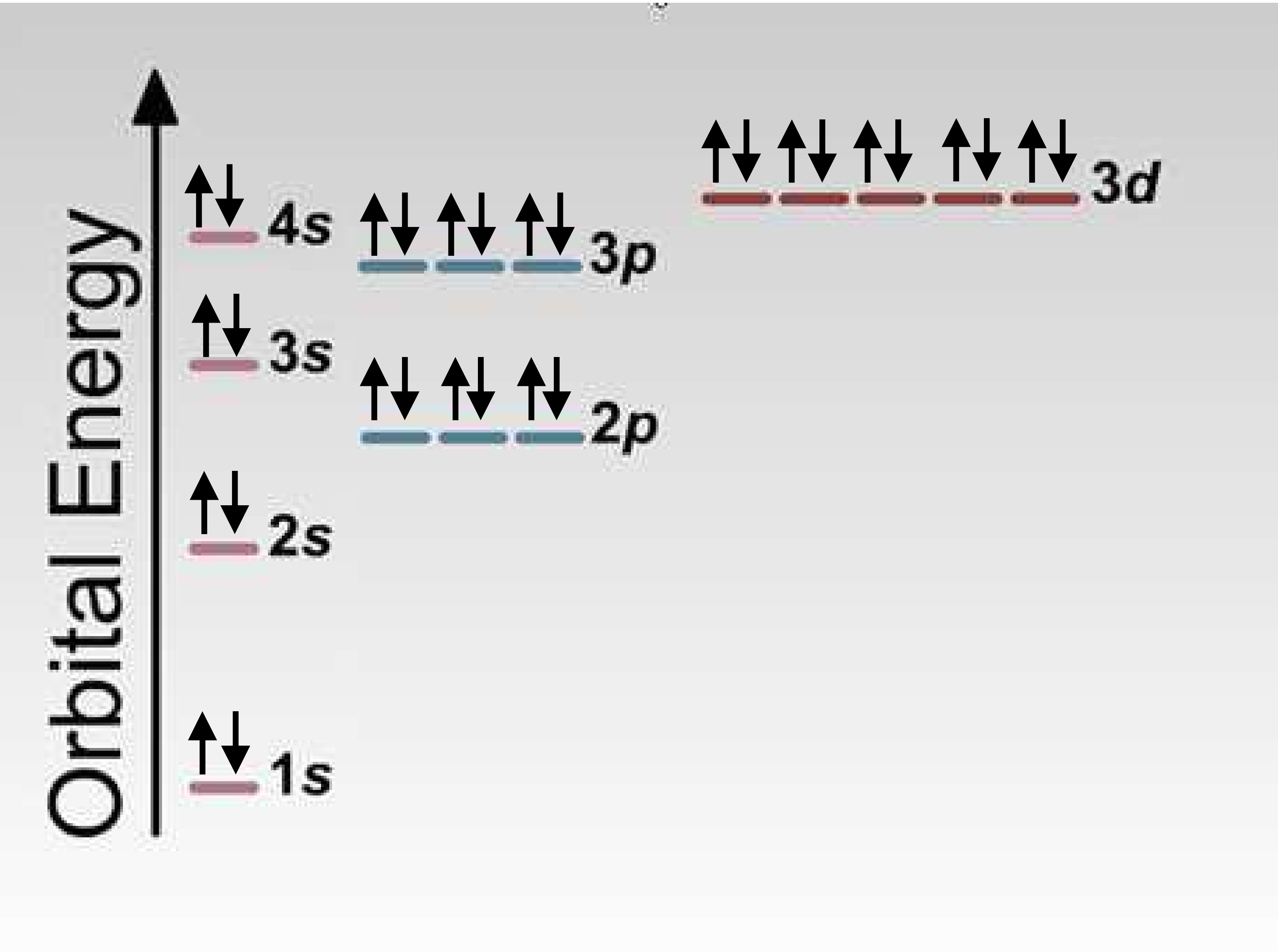
Relevant for electron configurations ***and*** *orbital diagrams:*

- Lower-energy orbitals fill before higher-energy orbitals.

Relevant only for orbital diagrams:

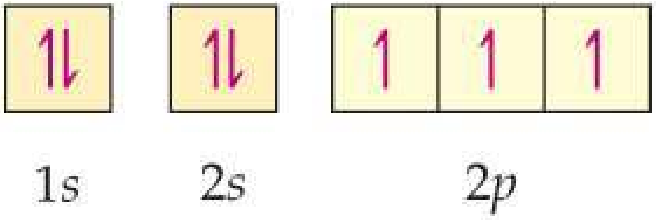
- ***Pauli exclusion principle.*** Orbitals can hold no more than two electrons each. When two electrons occupy the same orbital, they must have opposing spins..
- ***Hund's rule.*** When orbitals of identical energy are available, all of these are first occupied singly by electrons with parallel spins rather than electrons in pairs.

Writing Ground-State Electron Configurations

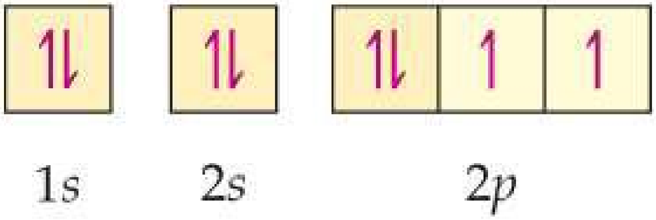


Writing Ground-State Electron Configurations

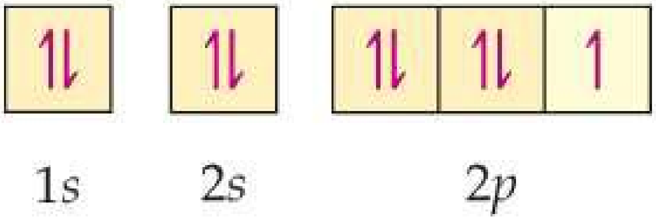
N (7) $1s^22s^22p^3$



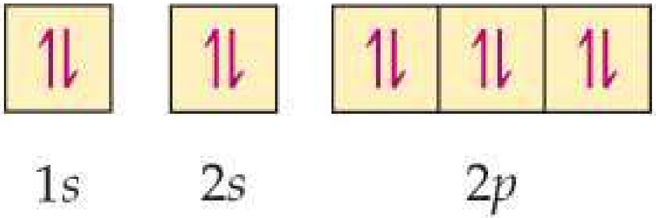
O (8) $1s^22s^22p^4$



F (9) $1s^22s^22p^5$



Ne (10) $1s^22s^22p^6$



With Neon, *n* = 2 shell is complete

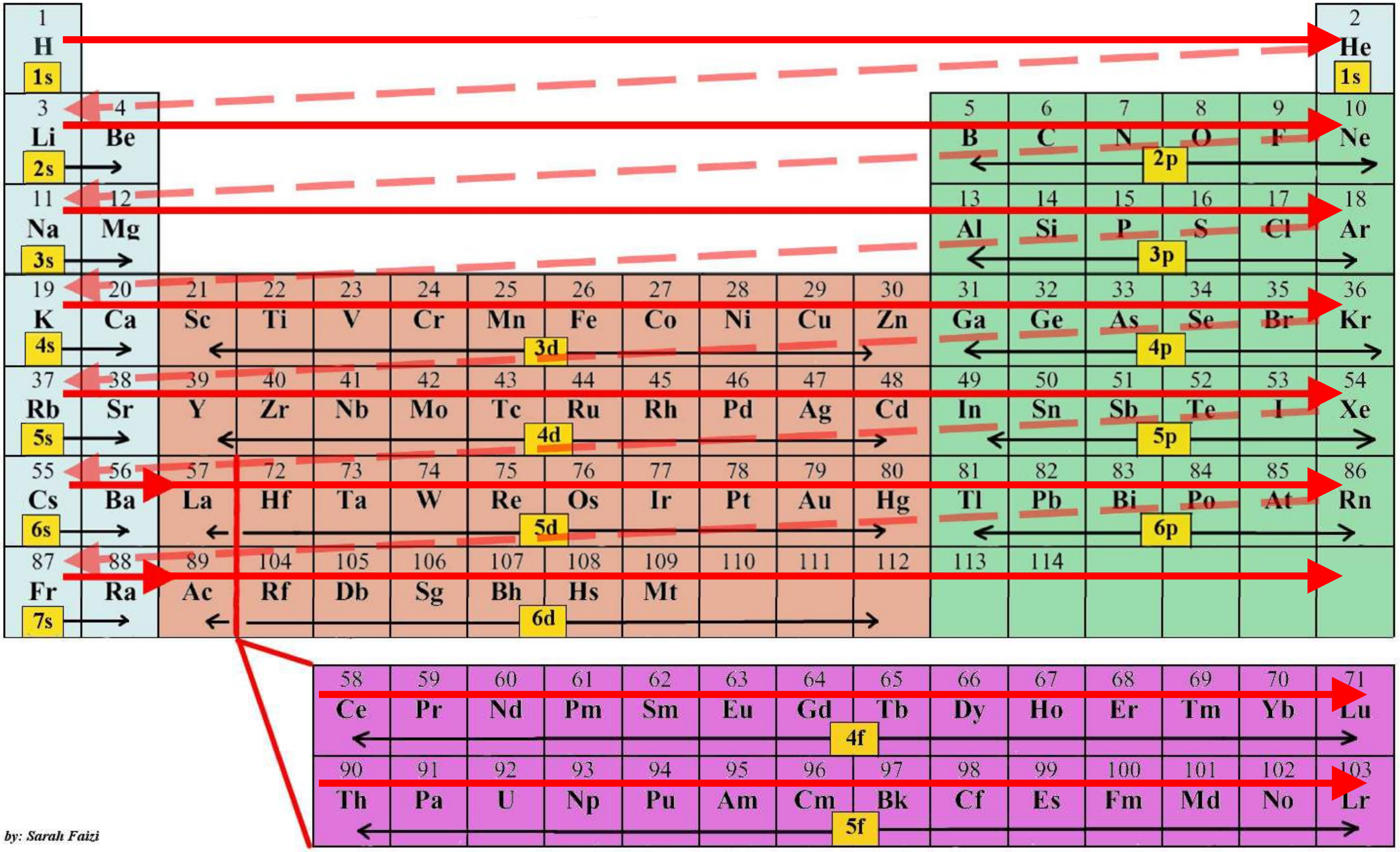
- Simple enough to populate the subshells until we come to 4*s*
- How do we know/remember that 4*s* electrons have lower energy than 3*d* electrons, etc?
- How do we know other cases when a subshell in a higher shell gets populated before a subshell in a lower shell?

Best way: Use the **Periodic Table**

Because:

- The origin of the periodic repetition of the properties lies in the electron configurations of the elements.
- Just as the electron configurations gives rise to the periodic table, **periodic table can give us the electronic configurations of the elements**.
- We just need to apply the aufbau principle, starting from the first element (H) onward and assign the electrons according to the “block” they belong to as we move from left to right and top to bottom, “reading” the table one element at a time until we arrive at the element whose configuration we want to find.

Order of filling subshells, by reading the periodic table like a book



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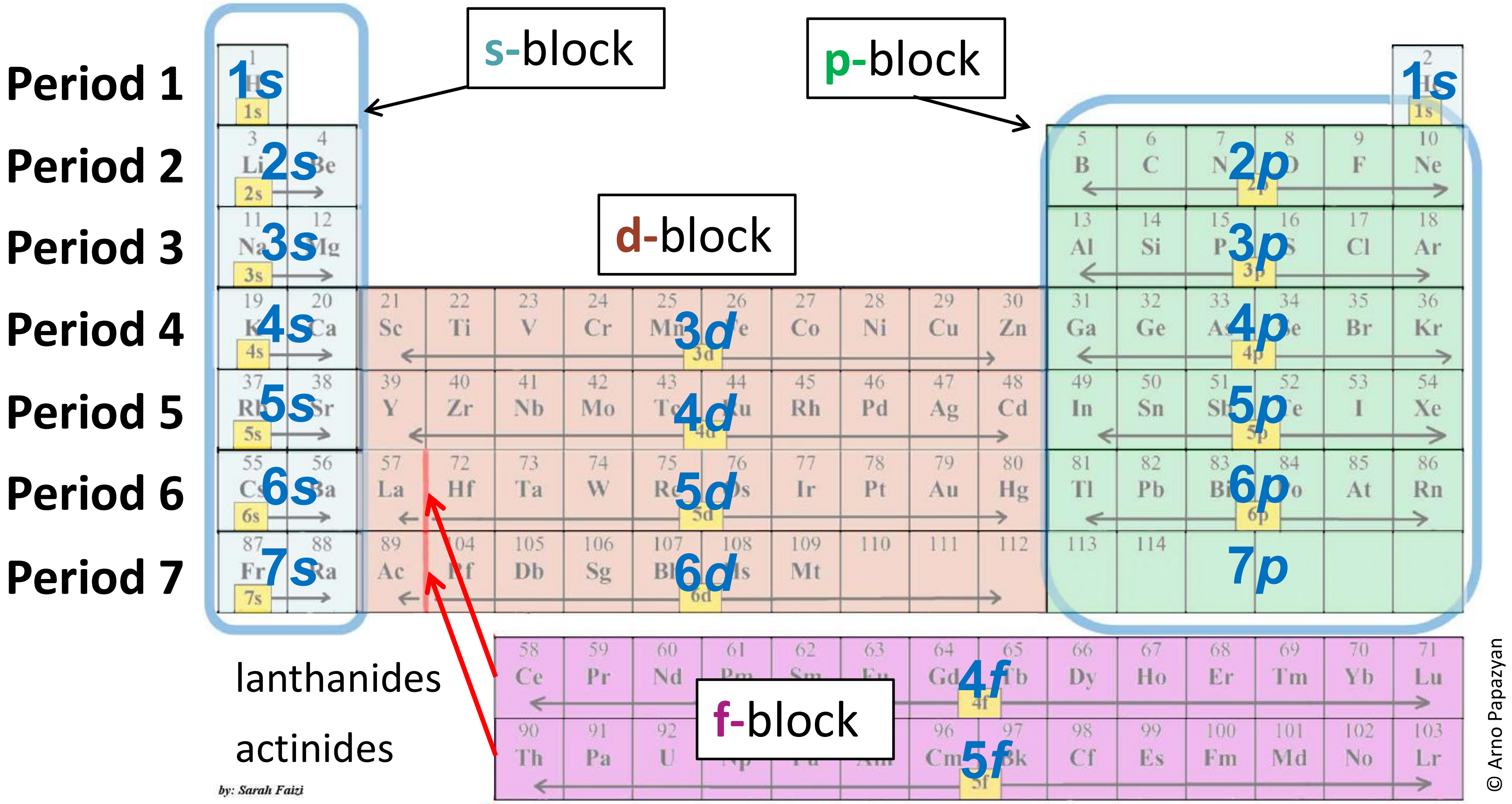
When building configurations:

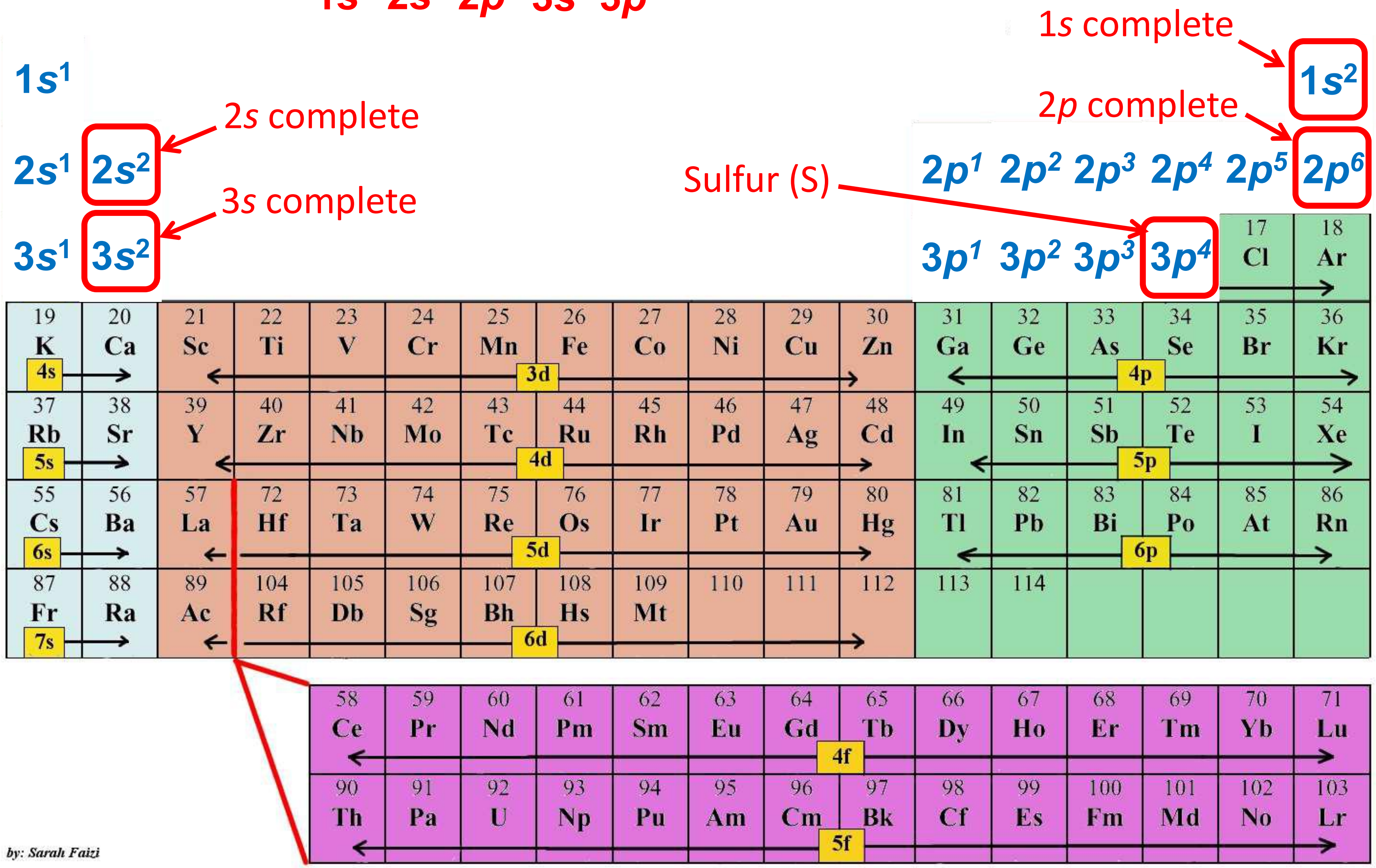
- **For s- and p-subshells: (Shell #) = (Period #)**
- **For d-subshells: (Shell #) = (Period #) – 1**
- **For f-subshells: (Shell #) = (Period #) – 2**



Example

What is the electron configuration of Sulfur (S)?

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$



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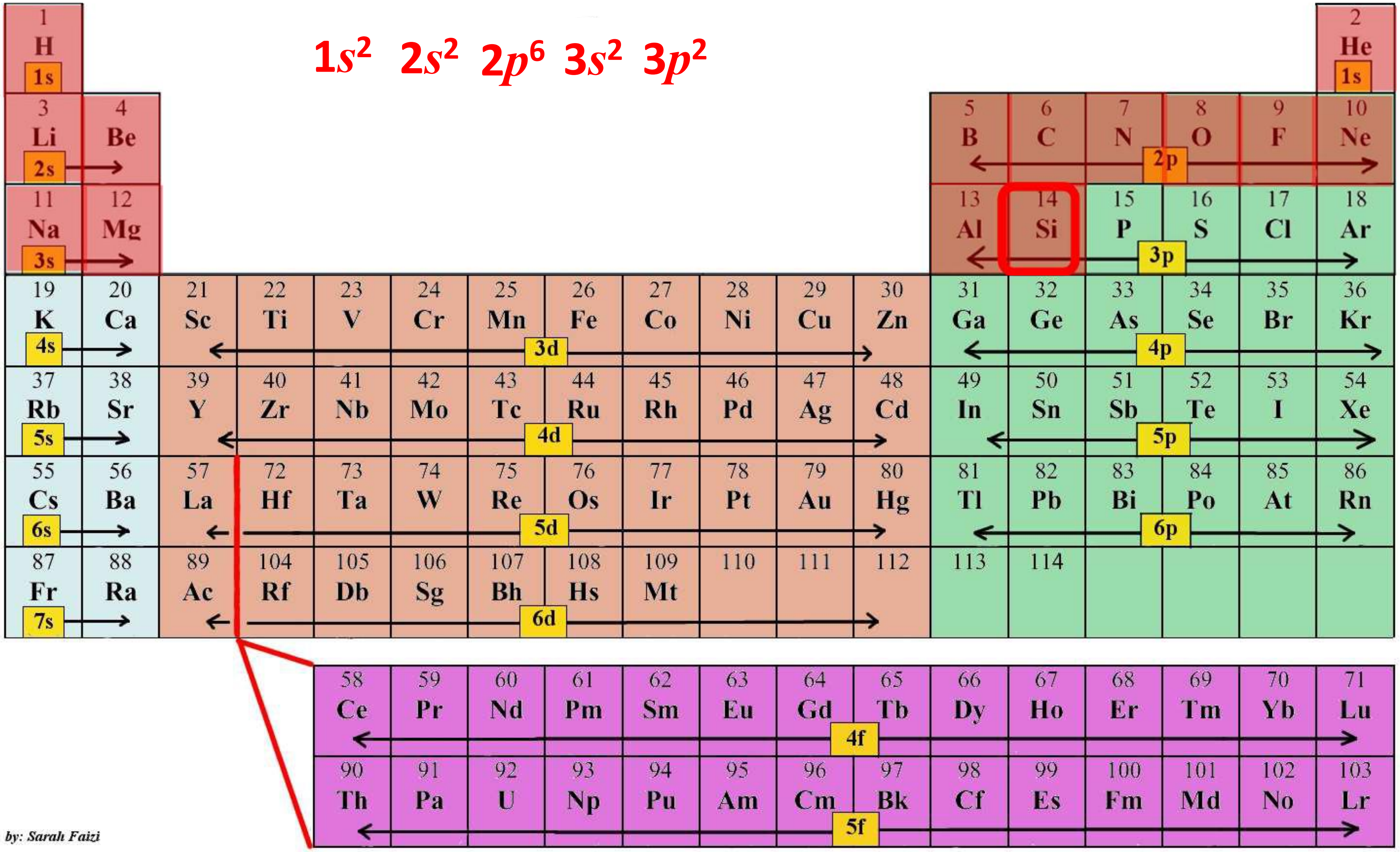
Example: Electron configuration of Si

$1s^2 \ \ 2s^2 \ \ 2p^6 \ \ 3s^2 \ \ 3p^2$



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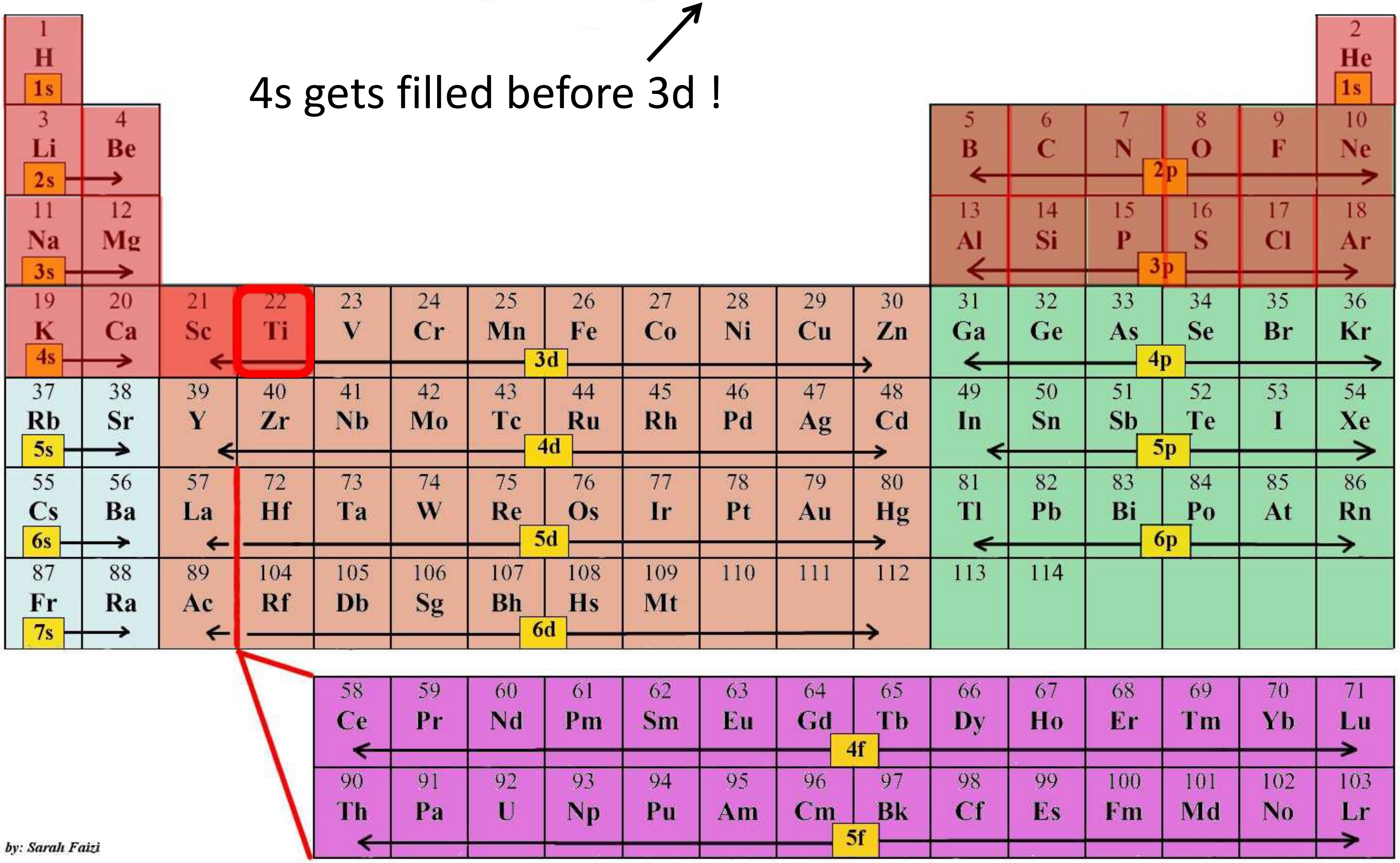
Example: Electron configuration of Ti

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^2$

4s gets filled before 3d !



1 H 1s																	2 He 1s
3 Li 2s	4 Be											5 B	6 C	7 N	8 O 2p	9 F	10 Ne
11 Na 3s	12 Mg											13 Al	14 Si	15 P	16 S 3p	17 Cl	18 Ar
19 K 4s	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe 3d	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se 4p	35 Br	36 Kr
37 Rb 5s	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru 4d	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te 5p	53 I	54 Xe
55 Cs 6s	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os 5d	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po 6p	85 At	86 Rn
87 Fr 7s	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs 6d	109 Mt	110	111	112	113	114				
				58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb 4f	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
				90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk 5f	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

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Abbreviated Electron Configuration

When writing electron configurations for elements beyond any noble gas, the electron configuration up to the previous noble gas can be abbreviated by the symbol for the noble gas in square brackets.

For sodium (Z=11; i.e. has 11 electrons)

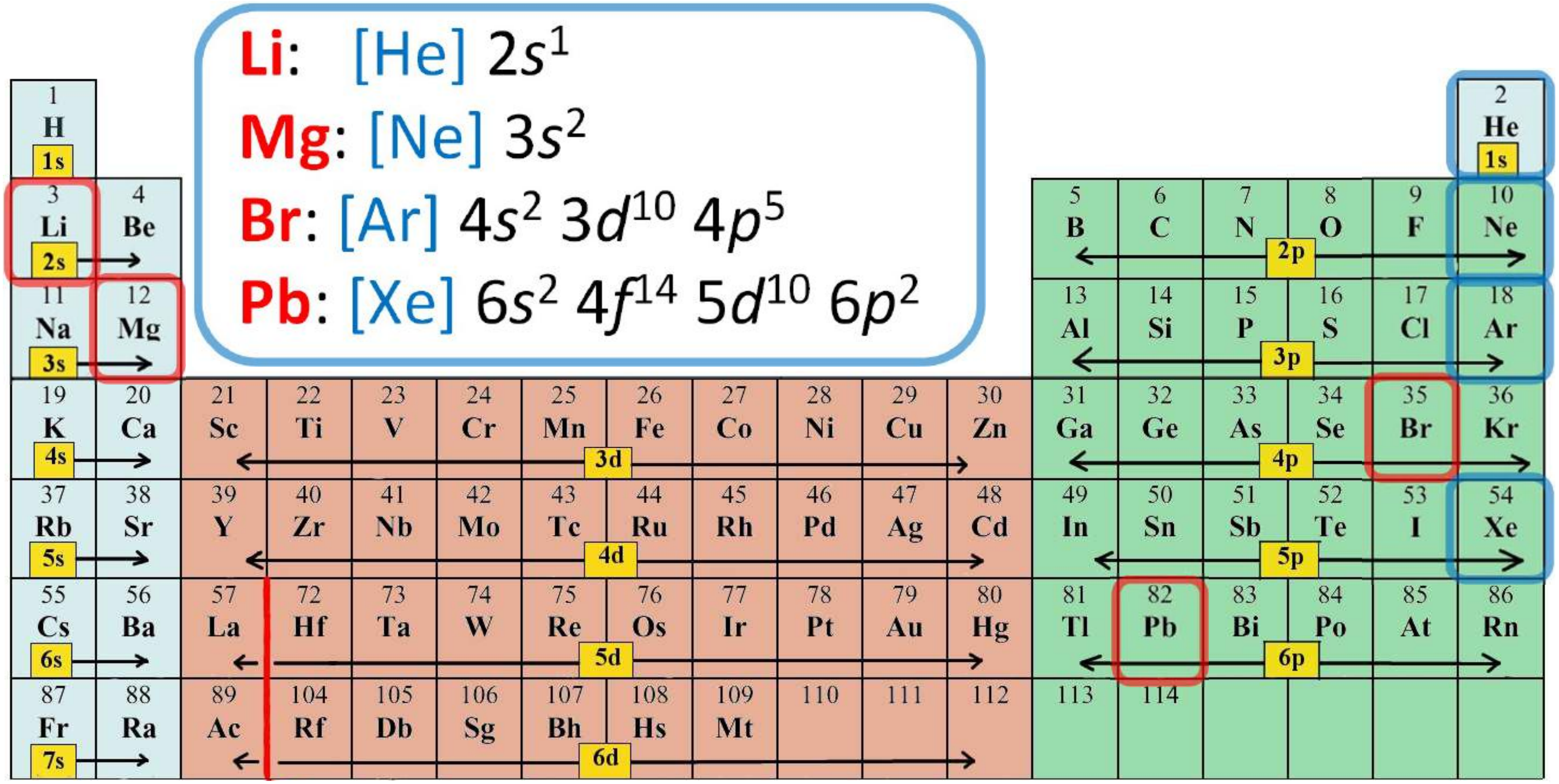
Na: $1s^2 2s^2 2p^6 3s^1$

Ne: $1s^2 2s^2 2p^6$

Na: $[\mathrm{Ne}]3s^1$

Abbreviated representation of electronic configurations

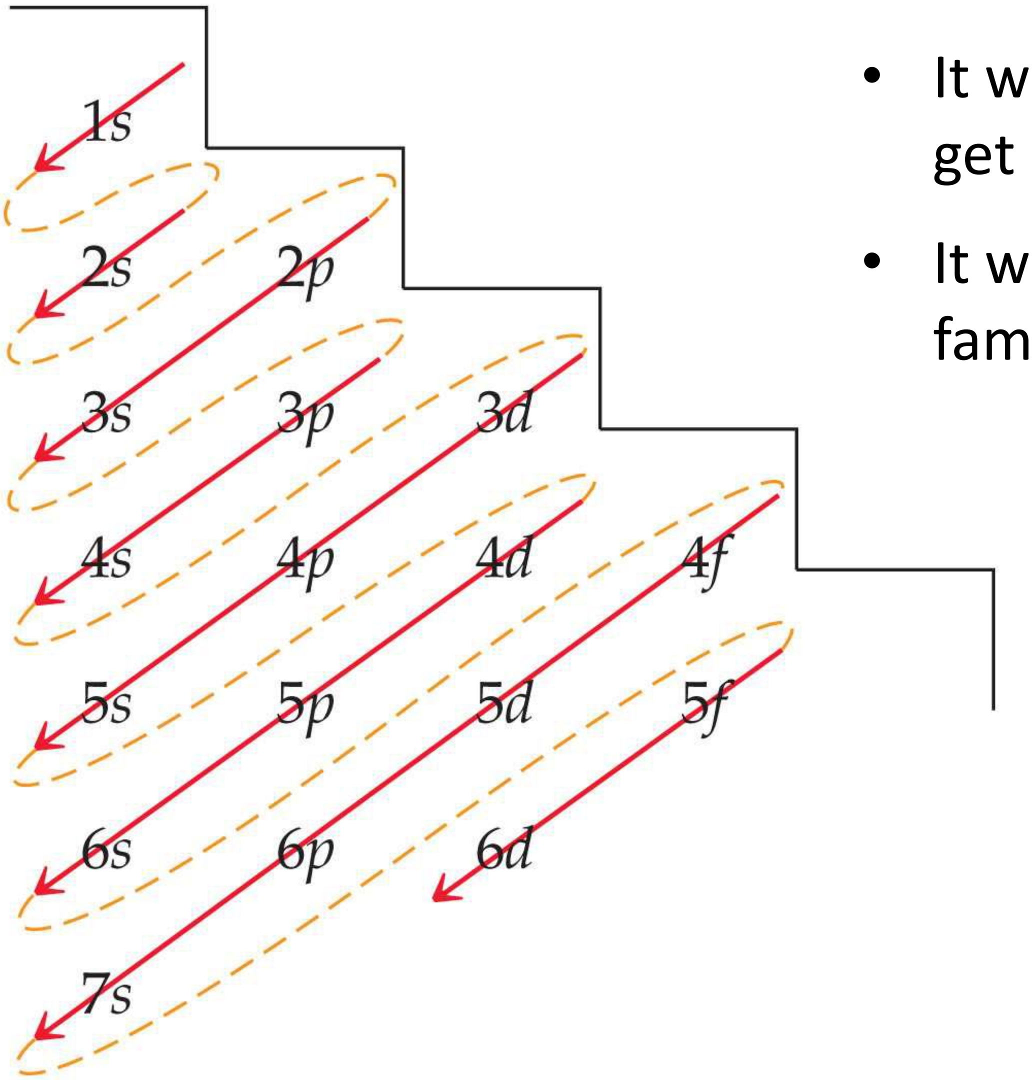
Only shows the configuration <u>beyond the last noble gas</u>.
-- with the last noble gas shown in <u>square brackets</u>



Li: [He] $2s^1$
Mg: [Ne] $3s^2$
Br: [Ar] $4s^2\ 3d^{10}\ 4p^5$
Pb: [Xe] $6s^2\ 4f^{14}\ 5d^{10}\ 6p^2$

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110	111	112	113	114				

Order of filling subshells; without a periodic table



You can use this, but:

- It won’t give you the insight you get by using the periodic table
- It won’t contribute to your getting familiar with the periodic table

Practice:

Check your solution on next page

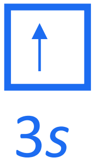
Use the Periodic Table to write the short electron configuration and short orbital diagram for each of the following

- Na (atomic no. 11)
- Te (atomic no. 52)
- Tc (atomic no. 43)

Practice: Use the Periodic Table to write the short electron configuration and short orbital diagram for each of the following

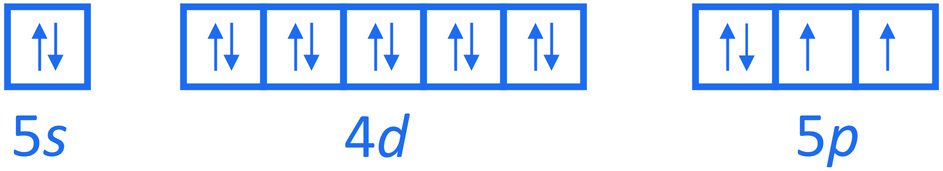
- Na (atomic no. 11)

$[\mathrm{Ne}]3s^1$



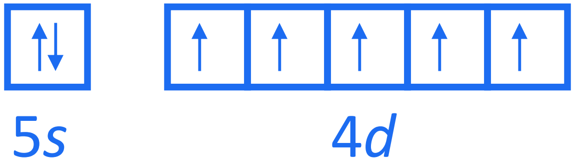
- Te (atomic no. 52)

$[\mathrm{Kr}]\ 5s^2\ 4d^{10}\ 5p^4$



- Tc (atomic no. 43)

$[\mathrm{Kr}]\ 5s^2\ 4d^5$

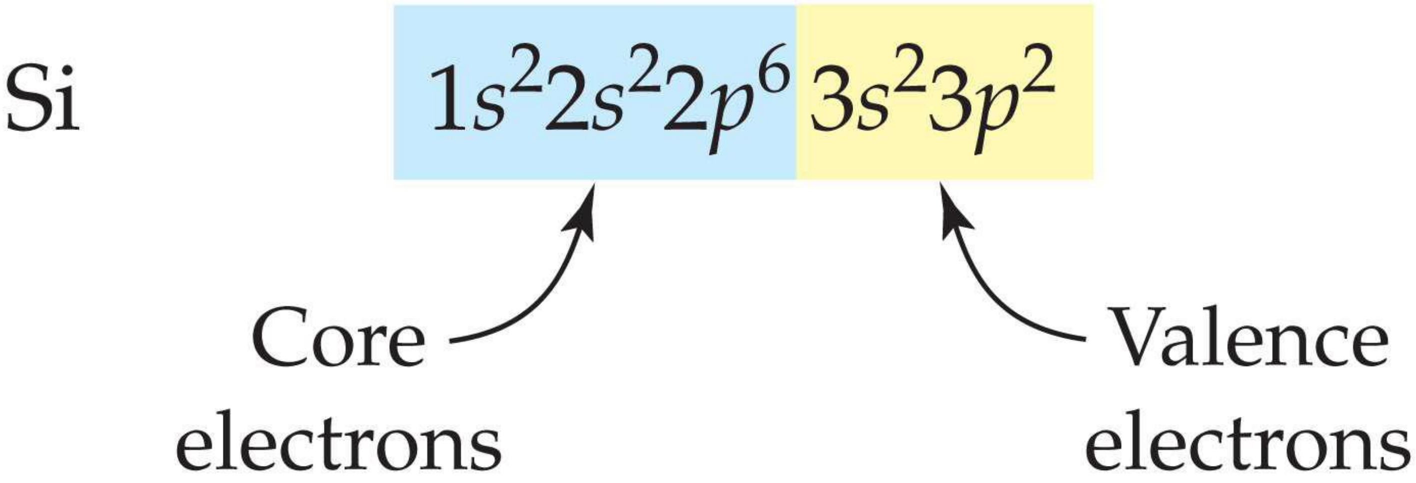


Valence Electrons and Core Electrons

- **Valence electrons** are the electrons in the outermost shell (the shell with the highest principal quantum number, *n*).
- These electrons are important because they are involved in chemical bonding.
- Electrons that are *not* in the outermost (valence) shell are called **core electrons**.

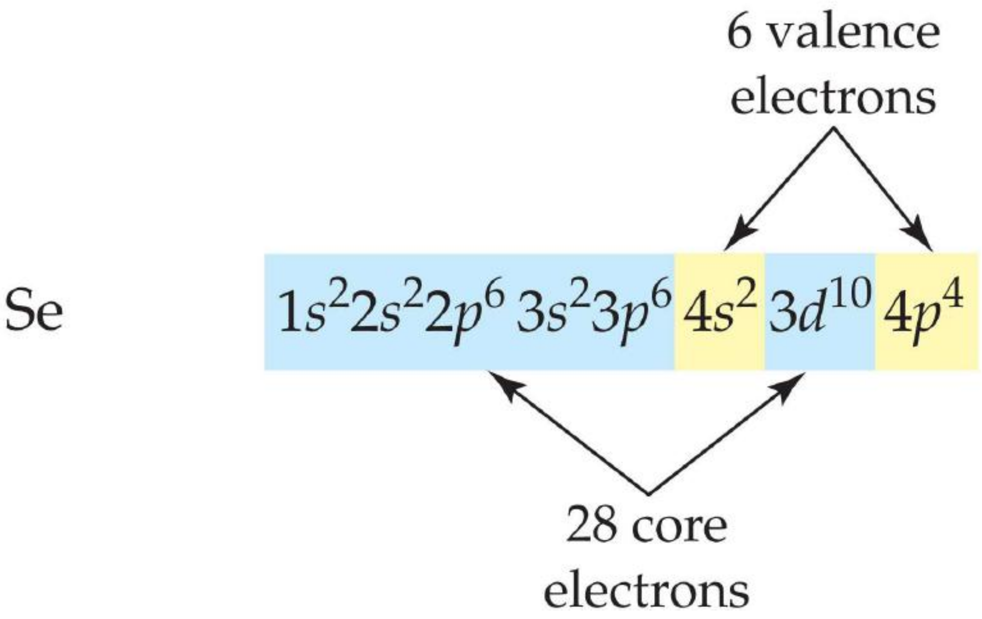
Valence Electrons and Core Electrons

Silicon (Z=14) has 4 valence electrons (those in the *n* = 3 shell) and 10 core electrons.



Valence Electrons and Core Electrons

Selenium (Z=34) has 6 valence electrons (those in the *n* = 4 shell).



6 valence electrons

Se $1s^22s^22p^6\,3s^23p^6\,4s^2\,3d^{10}\,4p^4$

28 core electrons

All other electrons, including those in the 3*d* orbitals, are core electrons.

Practice

Write the full and abbreviated electron configuration of Rb atom. Which electron (s) is/are the valence and core electrons

Practice

Write the full and abbreviated electron configuration of Rb atom. Which electron (s) is/are the valence and core electrons

Rb = 37 electrons

Full Configuration: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^1$

Abbreviated Configuaration: $[Kr]5s^1$

Valence electron: $5s^1$

Core electrons: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$

Practice (Check your solution on the next page)

Write the full ground state electron configuration of manganese, which electron (s) is/are the valence and core electrons

Practice (Check your solution on the next page)

Write the full ground state electron configuration of manganese, which electron (s) is/are the valence and core electrons

Mn 25 e^-

Full configuration $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^5$

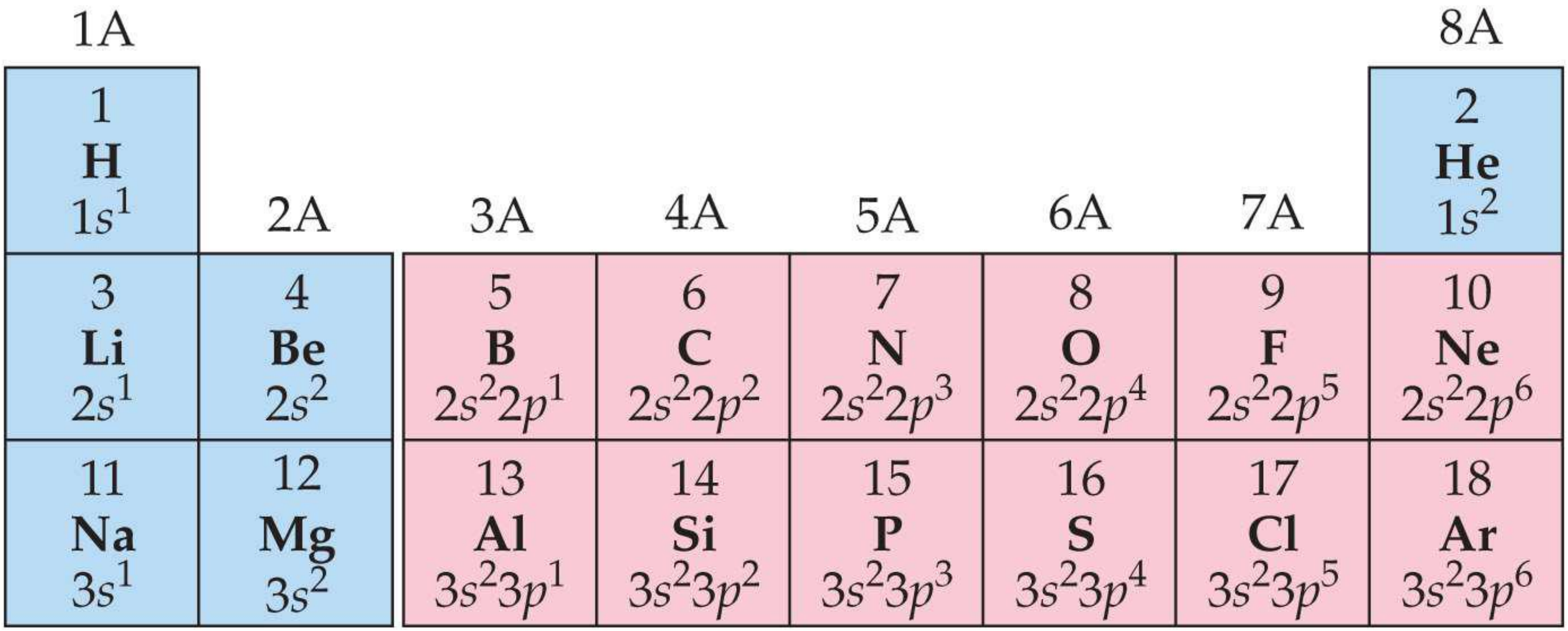
Abbreviated configuration $[Ar]\ 4s^2\ 3d^5$

Core e^- = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5$

Valence e^- $4s^2$

Electron Configurations of the Main Group Elements

The elements within a column of the periodic table all have the same number of valence electrons and similar valence electron configurations.



1A	2A	3A	4A	5A	6A	7A	8A
1 **H** $1s^1$							2 **He** $1s^2$
3 **Li** $2s^1$	4 **Be** $2s^2$	5 **B** $2s^22p^1$	6 **C** $2s^22p^2$	7 **N** $2s^22p^3$	8 **O** $2s^22p^4$	9 **F** $2s^22p^5$	10 **Ne** $2s^22p^6$
11 **Na** $3s^1$	12 **Mg** $3s^2$	13 **Al** $3s^23p^1$	14 **Si** $3s^23p^2$	15 **P** $3s^23p^3$	16 **S** $3s^23p^4$	17 **Cl** $3s^23p^5$	18 **Ar** $3s^23p^6$

Electron Configurations of the Main Group Elements

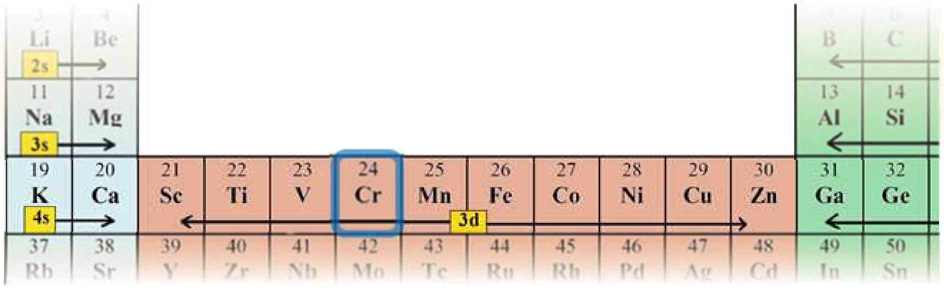
- The number of valence electrons for any main-group element is equal to the group number of its column. (Helium is an exception.)
  - e.g. Chlorine has 7 valence electrons because it is in the column with group number 7A.
- The row number in the periodic table is equal to the number of the highest principal shell (*n* value).
  - e.g. Chlorine is in row 3; its highest shell is the $n = 3$ shell.
- Remember that main-group elements are those in the two far left columns (1A, 2A) and the six far right columns (3A–8A) of the periodic table.

Electron Configurations of the Transition Elements

- The principal quantum number of the *d* orbital being filled across each row in the transition series is equal to the row number minus one. For example:
  - For the first transition series, the outer configuration is $4s^2 3d^x$ (x = number of *d* electrons).
- **Two exceptions: Cr is $4s^1 3d^5$ and Cu is $4s^1 3d^{10}$.**
- These exceptions occur because a filled or half-filled subshell (*d* or *s* in those cases) is particularly stable, and an electron can be "borrowed" from the valence *s*-subshell to attain them.

Irregularities in the buildup of electron configurations -- half-filled and filled subshells are favored

Cr and **Cu** are the important exceptions to remember

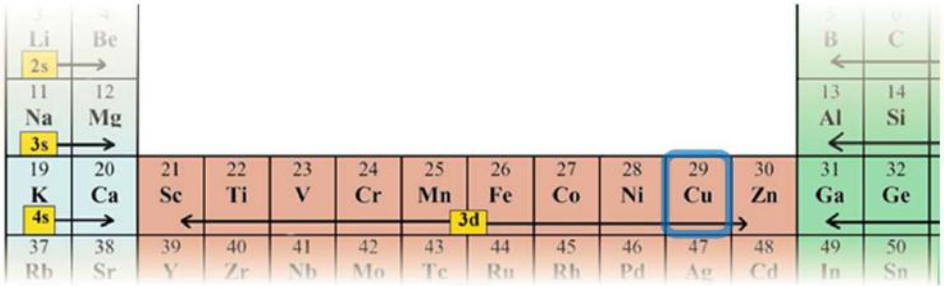


Cr:

Expected: [Ar] $4s^2\ 3d^4$

Actual: [Ar] $4s^1\ 3d^5$

Achieves half-filled *4s* and half-filled *3d* by shifting a *4s* electron to *3d*



Cu:

Expected: [Ar] $4s^2\ 3d^9$

Actual: [Ar] $4s^1\ 3d^{10}$

Achieves half-filled 4*s* & filled 3*d* by shifting a 4*s* electron to 3*d*

Irregular Electron Configurations in the electron configuration of the transition elements

Expected	Found Experimentally
Cr = [Ar] $4s^2$ $3d^4$	Cr = [Ar] $4s^1$ $3d^5$
Cu = [Ar] $4s^2$ $3d^9$	Cu = [Ar] $4s^1$ $3d^{10}$

Electron Configurations of the Ions Made by Elements

For an anion:

- Same as the neutral element with the same number of electrons as the anion.

N^{3-} : 1s^2 2s^2 2p^6 (with 3 more e^- ; same as Neon)

For a main-group cation:

- Same as the neutral element with the same number of electrons as the cation.

Ca^{2+} : 1s^2 2s^2 2p^6 (with 2 less e^- ; same as Argon)

Electron Configurations of the Ions Made by Elements

For a transition-metal cation:

Be careful!

- The electrons are first lost from the valence shell
- Only after the outermost, valence shell electrons are gone, should you remove electrons from the *d* subshell under it.

Ti : [Ar] $4s^2\ 3d^2$

Ti^{2+} : [Ar] $3d^2$

Ti^{4+} : [Ar]

Zn : [Ar] $4s^2\ 3d^{10}$

Zn^{2+} : [Ar] $3d^{10}$

Practice (Check your solution on next page)

Write the electron configuration of these Ions

S^{2-} ion

Mg^{2+} cation

Mn^{2+} ion

Practice (Check your solution on next page)

Write the electron configuration of these Ions

S atom = $1s^2\,2s^2\,2p^6\,3s^2\,3p^4$

S^{2-} anion = $1s^2\,2s^2\,2p^6\,3s^2\,3p^6$

Mg atom = $1s^2\,2s^2\,2p^6\,3s^2$

Mg^{2+} cation = $1s^2\,2s^2\,2p^6$

Mn $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^2\,3d^5$

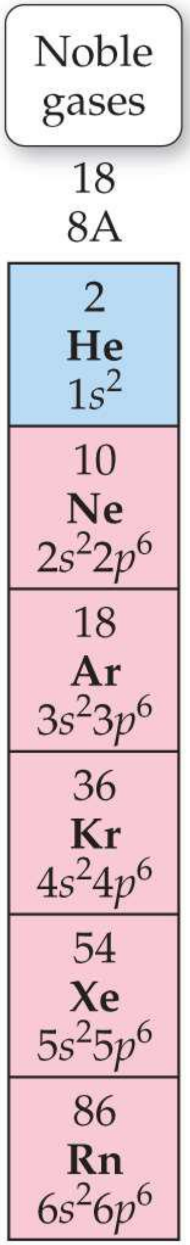
Mn^{2+} cation $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^5$

The Explanatory Power of the Quantum-Mechanical Model

- *The chemical properties of elements are largely determined by the number of valence electrons they contain*.
- Their properties vary in a periodic fashion because the number of valence electrons is periodic.

The Noble Gases

- Noble gas electron configurations are such that removing or adding an electron costs too much energy to be energetically favorable.
- This has the same effect as the configuration being particularly stable (i.e. “as if it is”)
- The noble gases are chemically stable, and thus relatively inert or nonreactive as accounted for by the quantum model.
- Elements with electron configurations close to the noble gases are the most reactive because they can attain noble gas electron configurations by losing or gaining a small number of electrons (again, this explanation is not fundamental, and should be understood as “as if that’s why”)



Noble gases

18
8A

2
He
$1s^2$

10
Ne
$2s^22p^6$

18
Ar
$3s^23p^6$

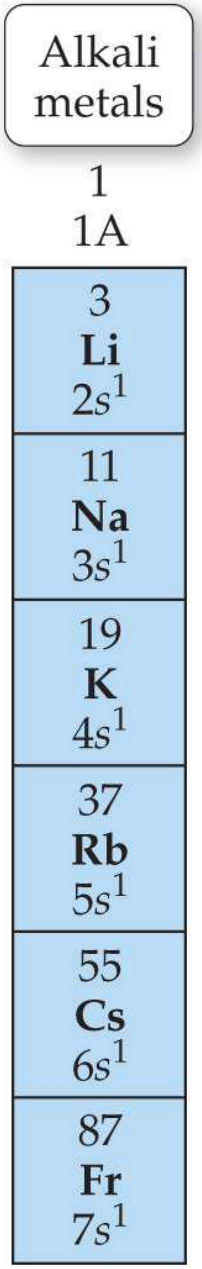
36
Kr
$4s^24p^6$

54
Xe
$5s^25p^6$

86
Rn
$6s^26p^6$

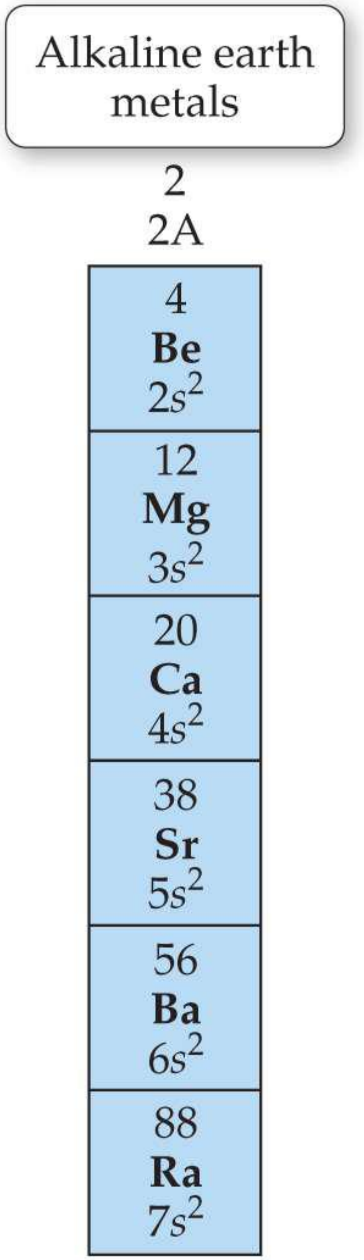
The Alkali Metals

- Alkali metals (Group 1) are among the most reactive metals since their outer electron configuration (ns^1) is 1 electron beyond a noble gas configuration.
- If they can react to lose the electron, they attain a noble gas configuration.
- This explains why the Group 1 metals tend to form 1+ cations.



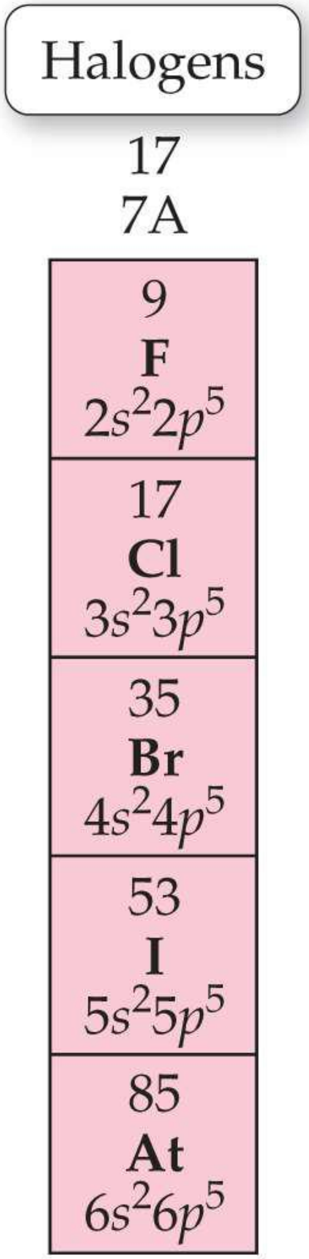
The Alkaline Earth Metals

- The alkaline earth metals (Group 2) all have electron configurations ns^2 and are therefore 2 electrons beyond a noble gas configuration.
- In their reactions, they tend to lose 2 electrons, forming 2+ ions and attaining a noble gas configuration.



The Halogens

- The halogens (Group 7) all have ns^2np^5 electron configurations and are therefore 1 electron short of a noble gas configuration.
- In their reactions, halogens tend to gain 1 electron, forming 1− ions and attaining a noble gas configuration.



Trends in the periodic table

We will study the periodic trends of :

Atomic Radius

- Radius of the outermost occupied shell (valence shell)

Ionization Energy

- Energy required to remove an electron from the valence shell of a gaseous atom

$X(g) \rightarrow X^+(g) + e^-$ ΔE = ionization energy of X

$Mg\ (g) \rightarrow Mg^+\ (g)\ + e^-$ $\Delta E = 735$ kJ/mol

To understand trends, we need to remember:

Protons in the nucleus are (+) charged

Electrons in the surrounding shells are (–) charged

Protons and electrons attract

Stronger attraction pulls electrons closer to the nucleus, making the radius of the orbital smaller

Stronger attraction makes it harder to remove an electron from the atom, making the ionization energy higher

Proton-electron attraction gets weaker with distance

Vertical trends in the periodic table

Going downward in a group:

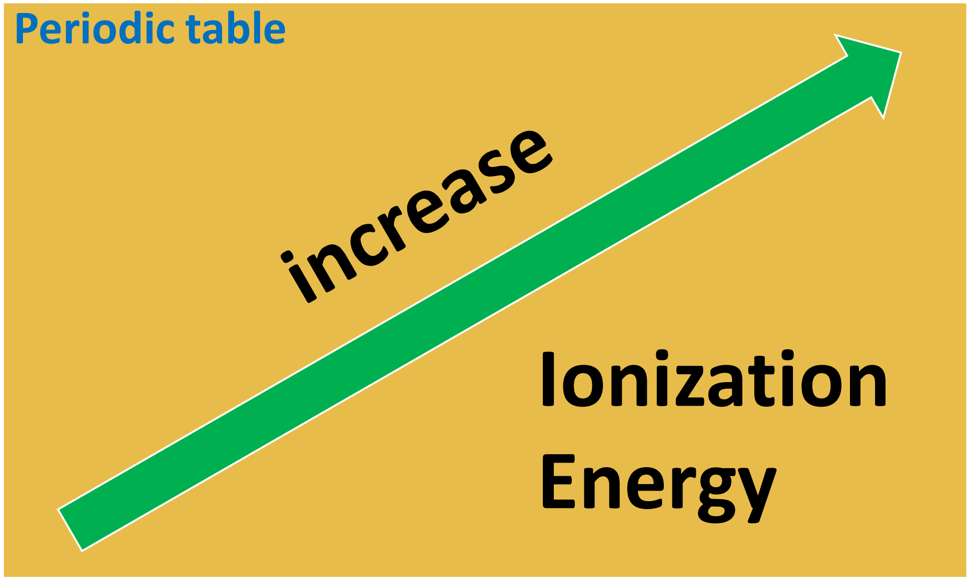
- Each time we go down in the periodic table, a new valence shell starts getting populated
- The valence shell is the farthest from the nucleus
  - ➢**The radius of the atom increases**
- Since the distance from the nucleus increases, the attraction to the nucleus decreases
  - ➢**Ionization energy decreases**

Horizontal trends in the periodic table

Going from left to right in a period:

- Electrons are added to the same shell, and protons are added to the nucleus
- Increased attraction to the nucleus pulls the electrons in
  - ➢ smaller radius
- Increased attraction to the nucleus makes it harder to remove an electron from the valence shell
  - ➢ Increasing ionization energy

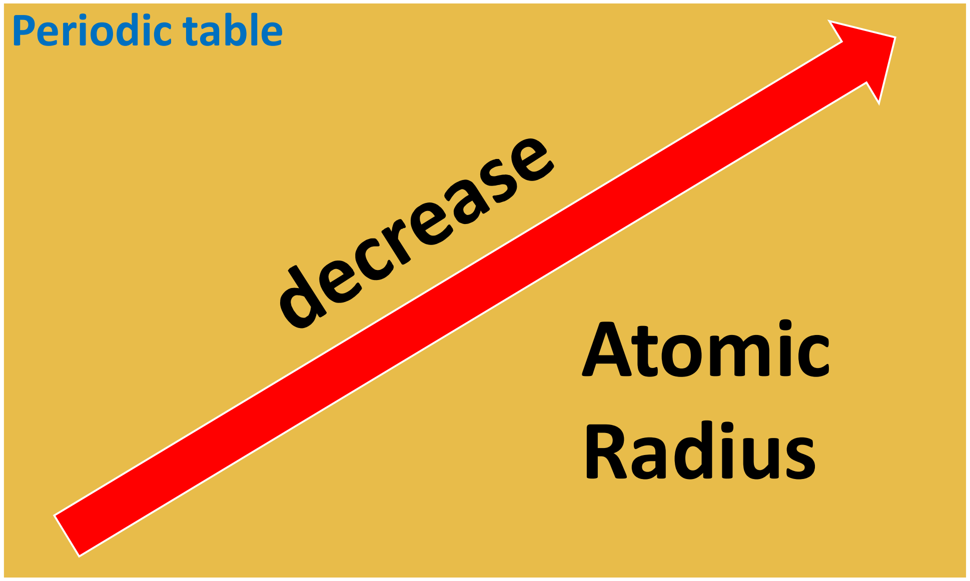
Ionization Energy and Atomic Radius have opposite trends



Periodic table

increase

Ionization Energy



Periodic table

decrease

Atomic Radius

Using metallic character to remember trends

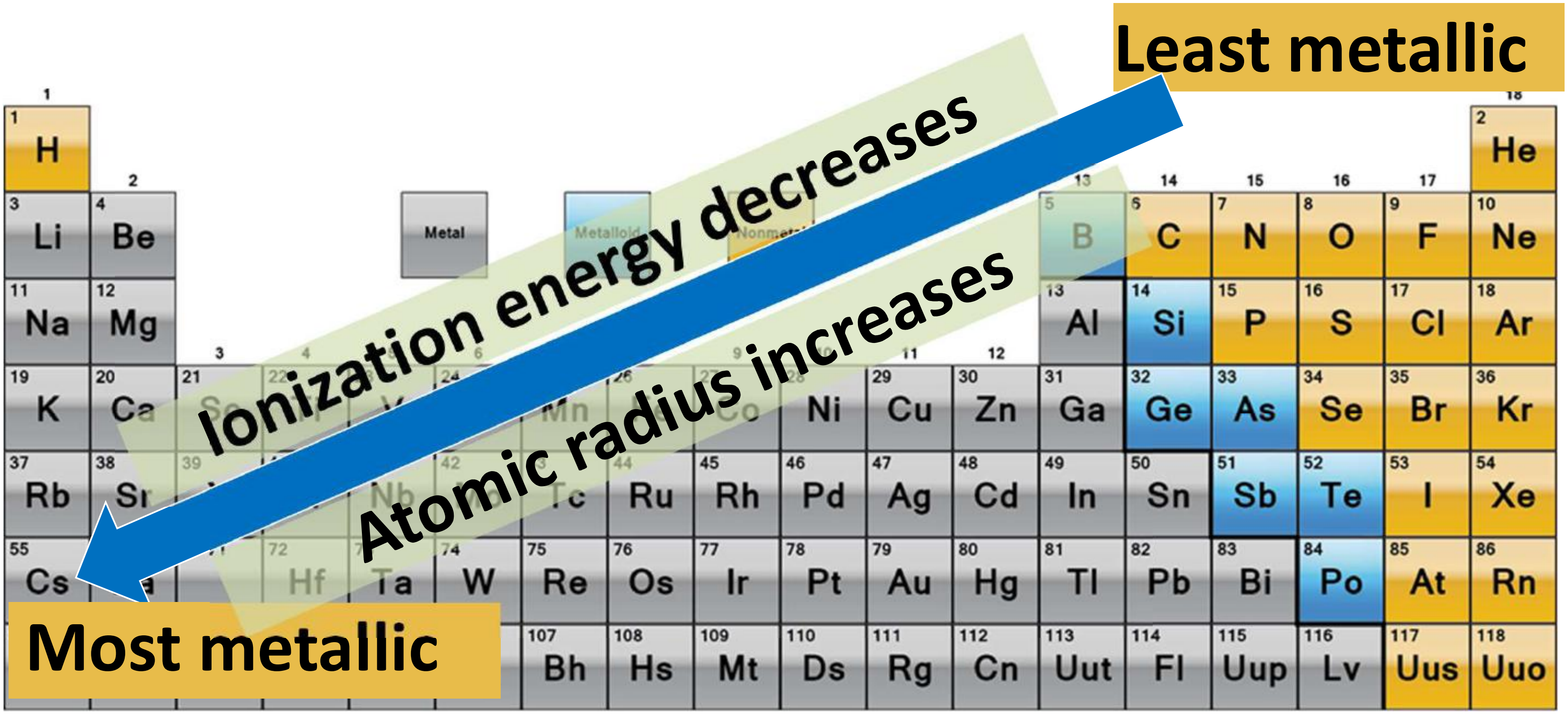
- Where in the periodic table are the metals?
  - To the left and bottom (away from top-right corner)

- What’s the most important characteristic of metals?
  - They conduct electricity
  - Because their valence electrons are “loose” (not strongly bound to the atoms)
  - So it’s easy to remove electrons from metal atoms (low ionization energy)

Low ionization energy leads to metallic character

More metallic means “lower ionization energy”

And if we remember that atomic radius trend is the opposite of ionization energy, we are set!



Least metallic

Ionization energy decreases

Atomic radius increases

Most metallic