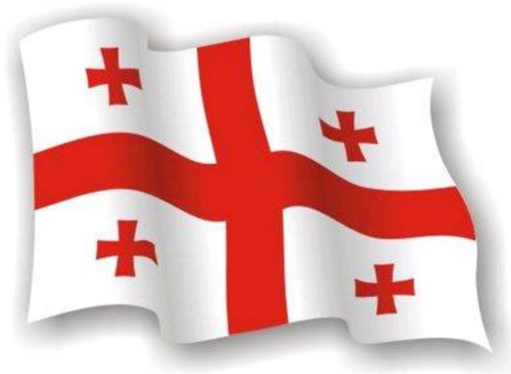


Mitglied der Helmholtz-Gemeinschaft

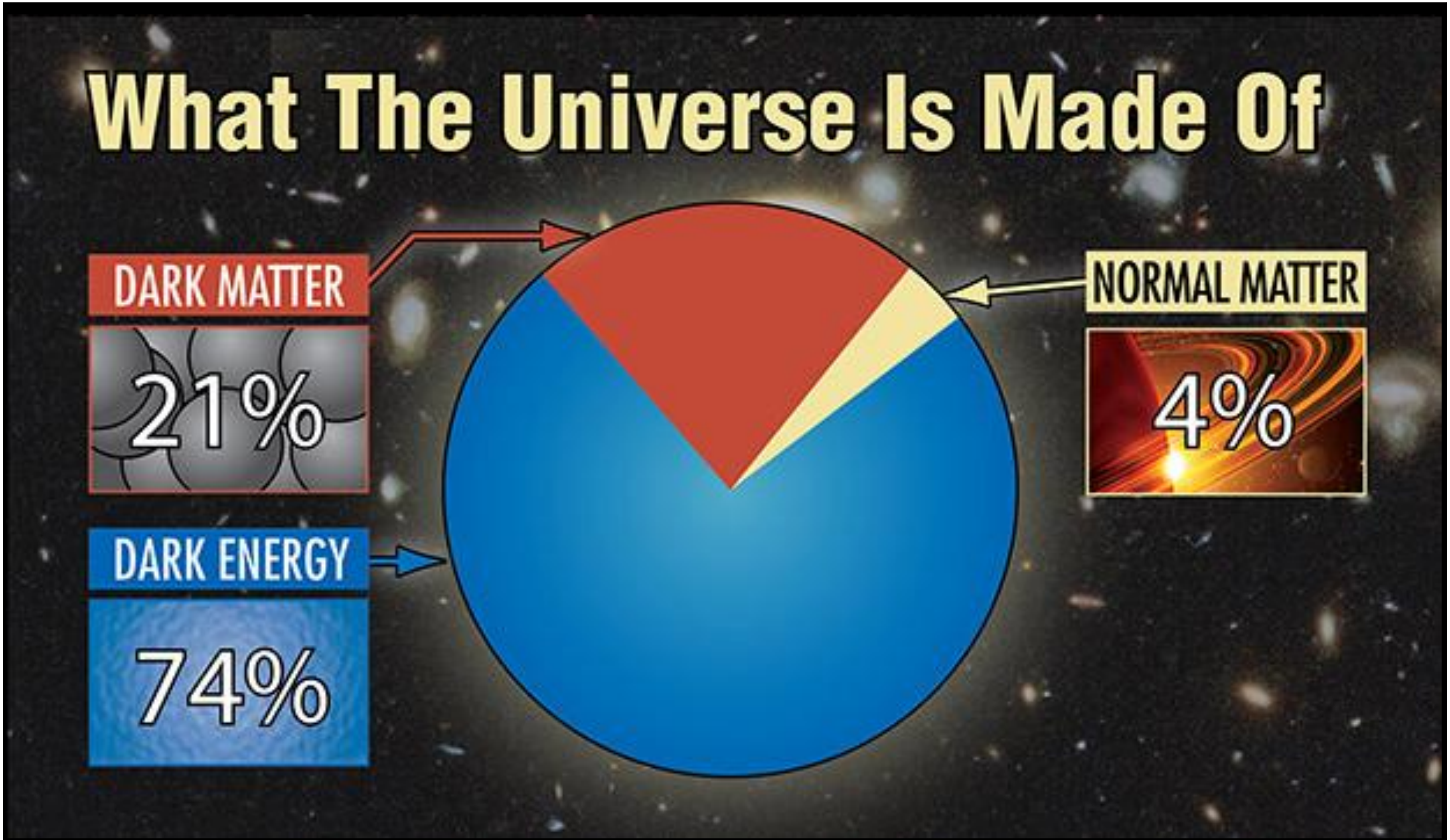
Georgian-German Science Bridge

Structure of Matter (SoM): Lecture 1: Atoms

October 15, 2013 | Hans Ströher (Forschungszentrum Jülich)

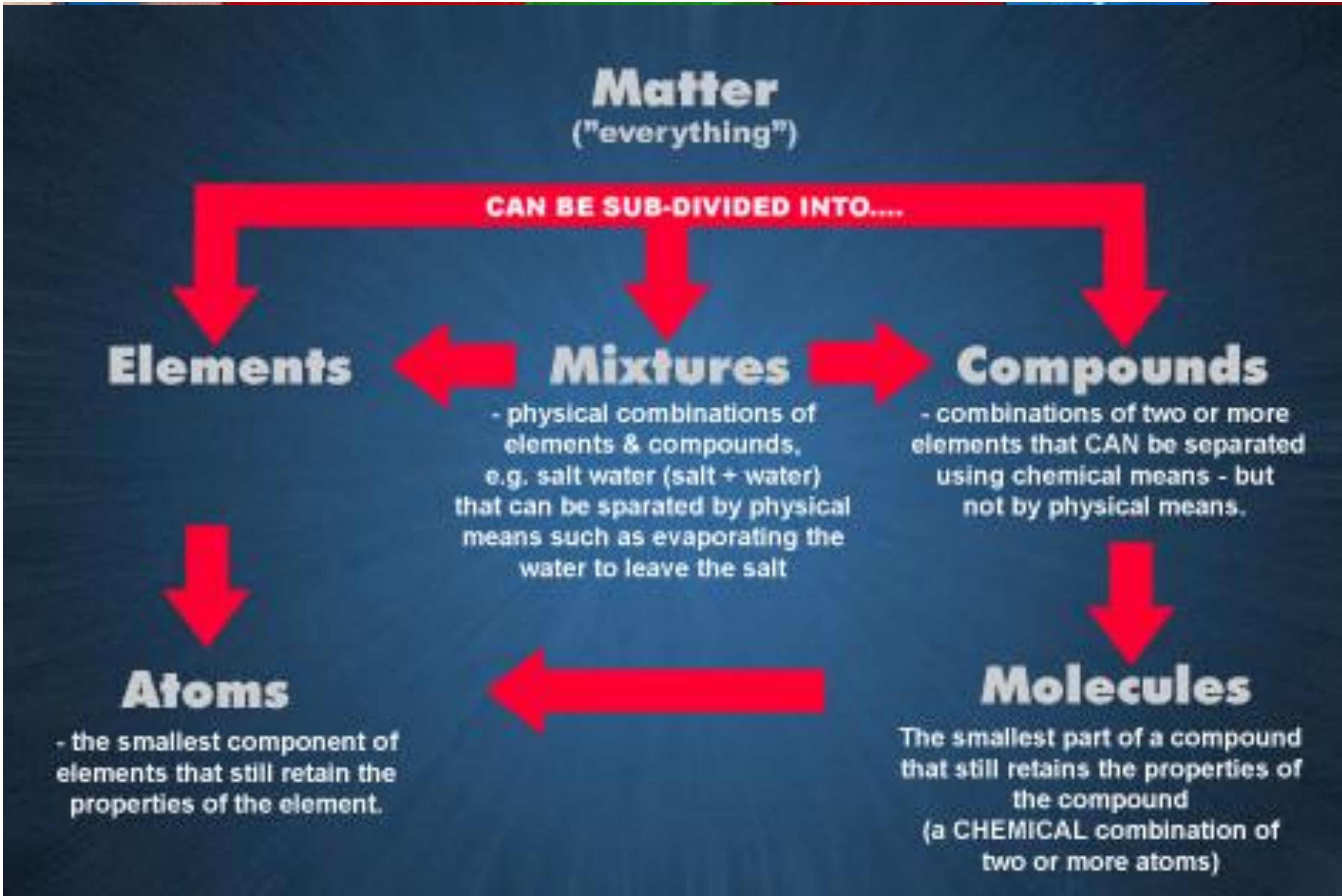
“MAKE EVERYTHING AS SIMPLE AS POSSIBLE, BUT NOT SIMPLER.”

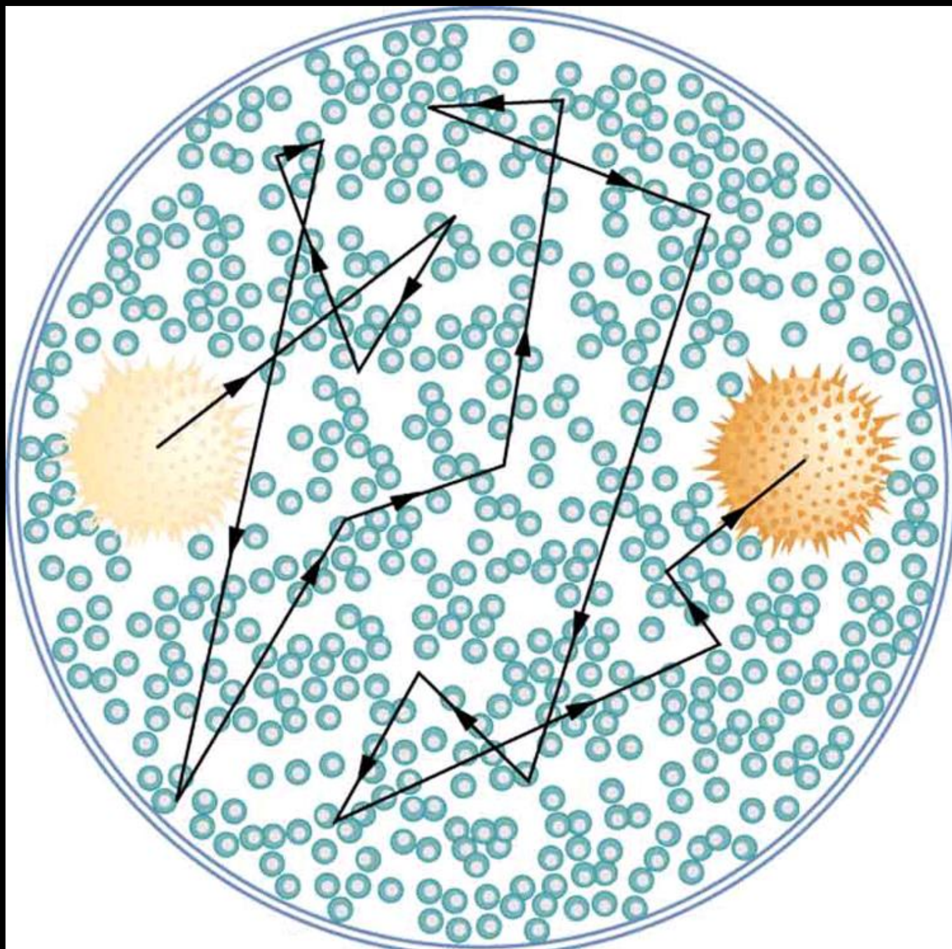
Albert Einstein

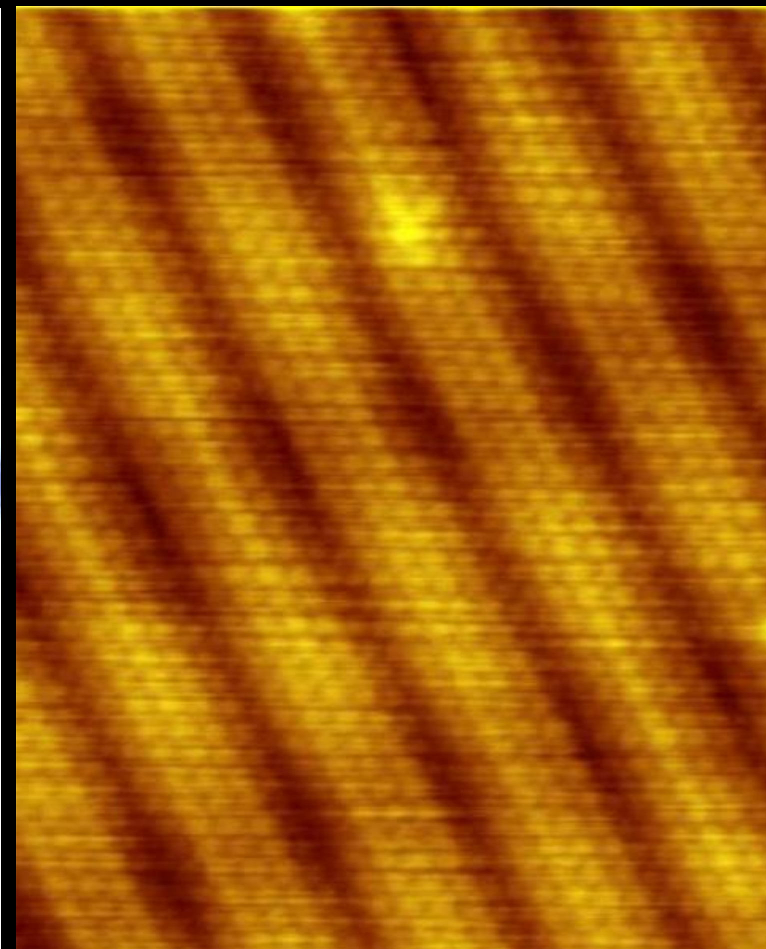


Lecture is only about these 4% …

Lecture 1 – Atoms – Introduction





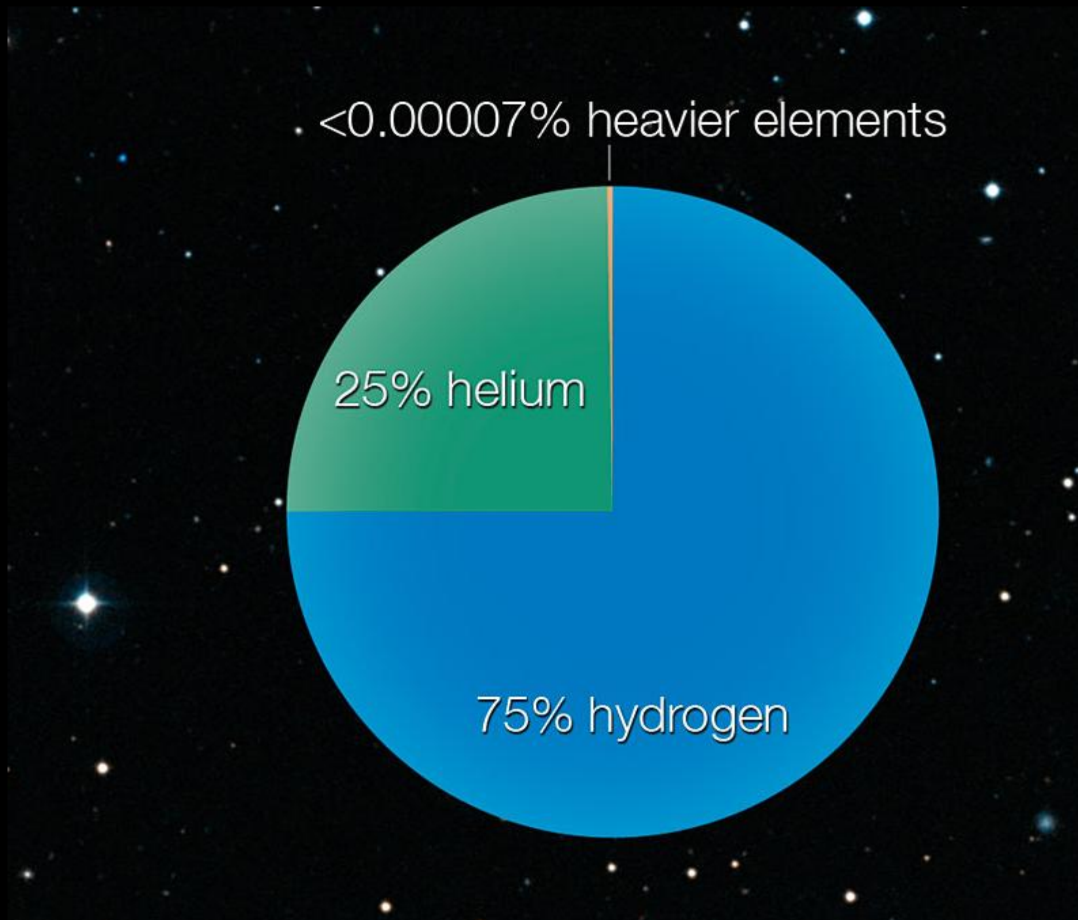


Discovery of the Atom

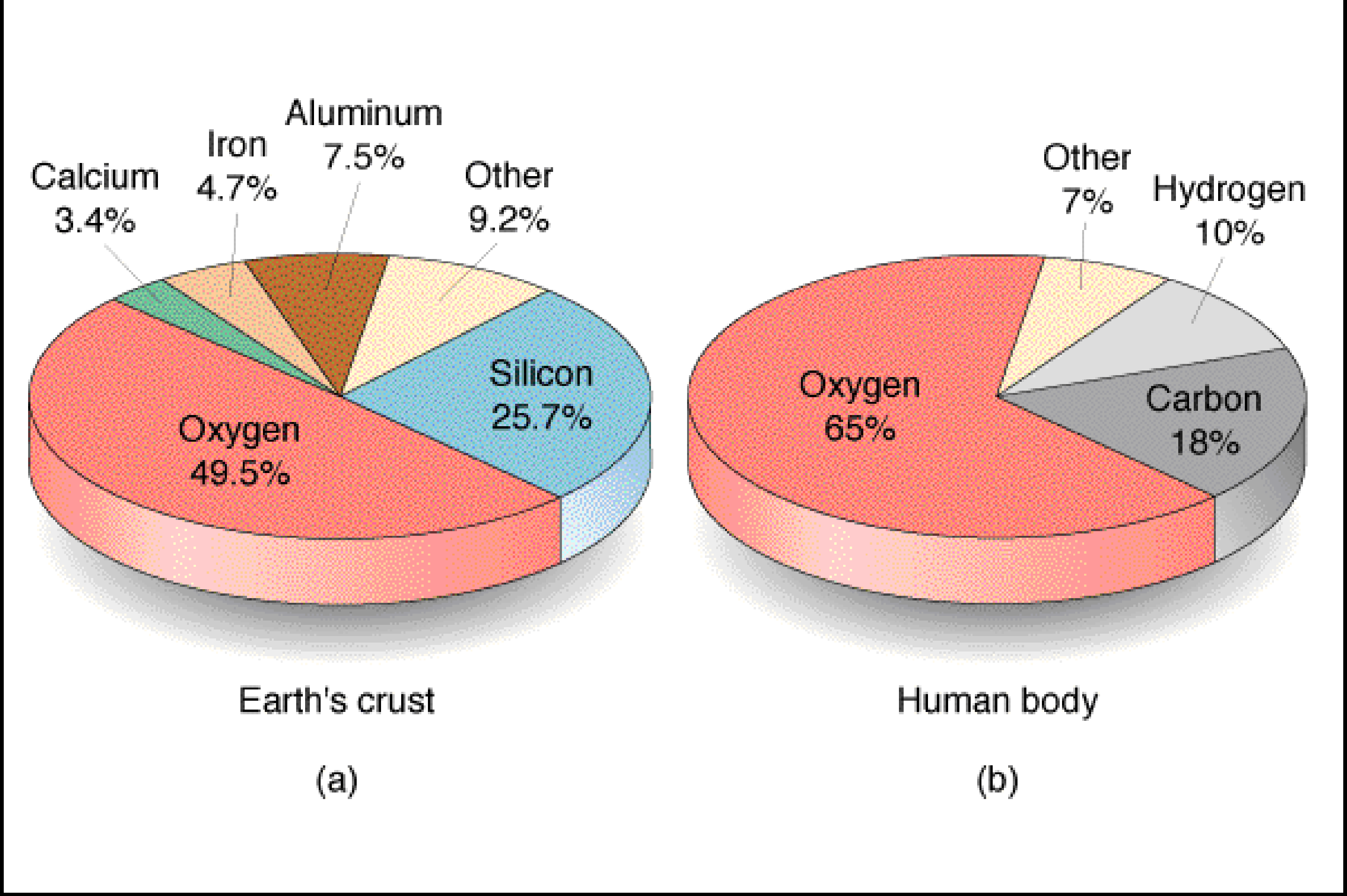
Lecture 1 – **Atoms** – Introduction

All matter is composed of **atoms**, the different kinds being known as **elements**. There are 114 (+ x) elements identified, but only a few dozen are found in biological systems.

Lecture 1 – Atoms – Introduction



Universe: Hydrogen and Helium

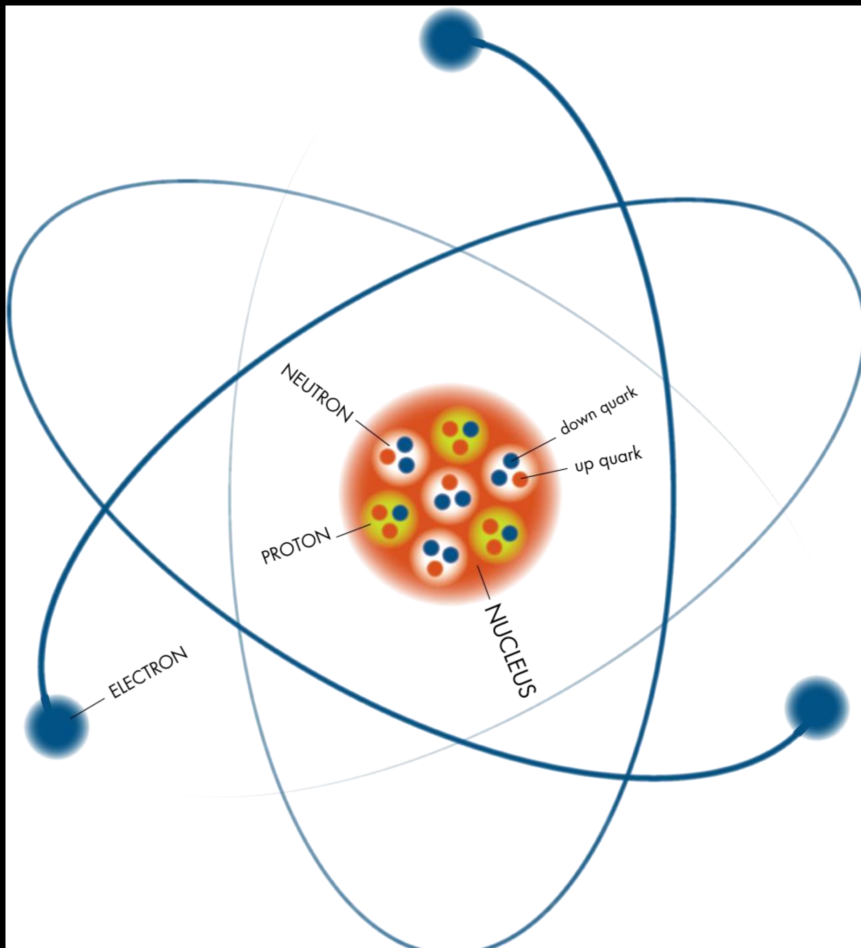


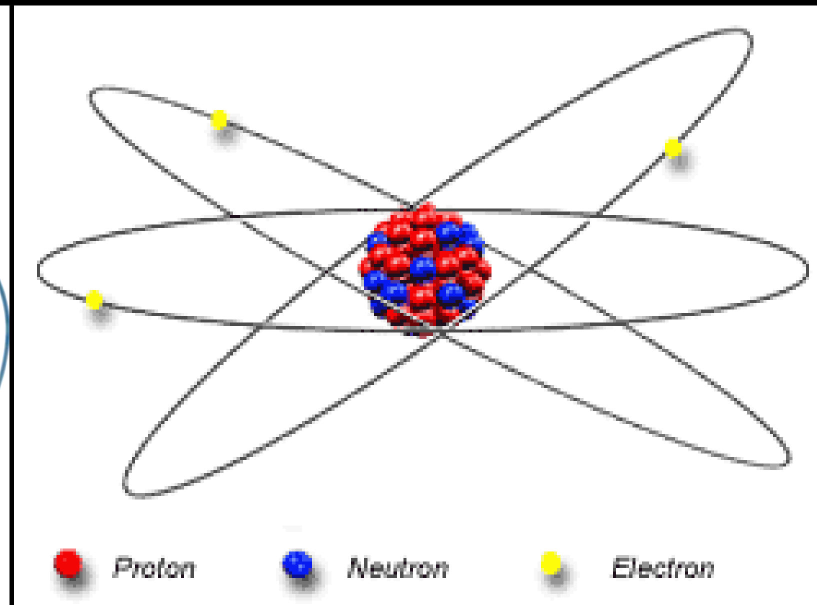
Abundances (Weight)

Lecture 1 – Atoms – Introduction

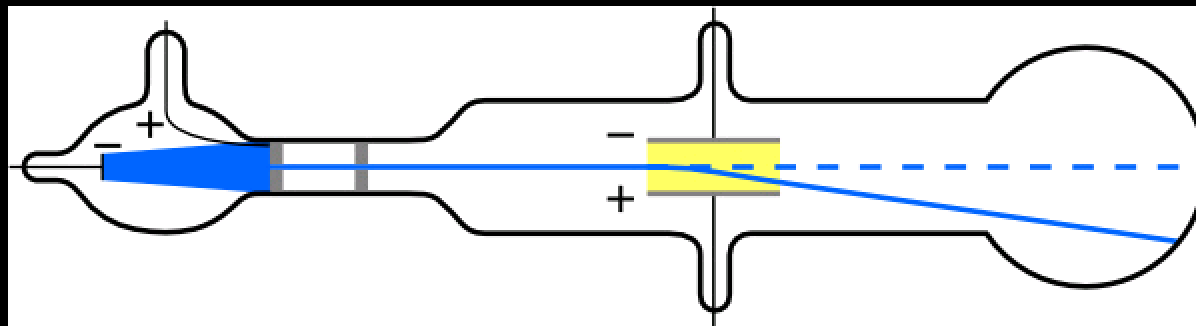
All atoms are constructed similarly:

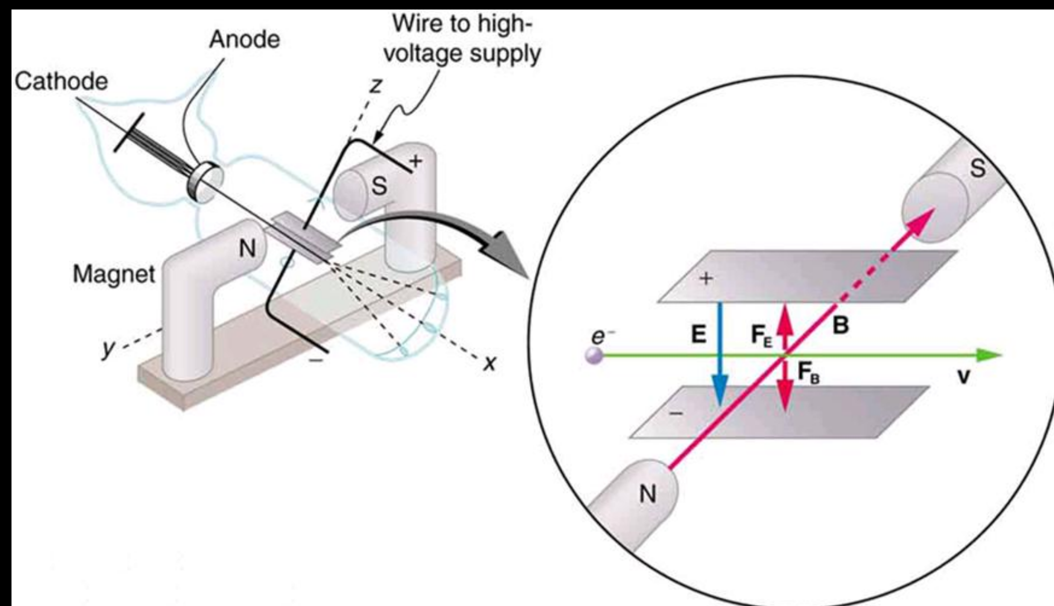
- There is a **nucleus** with **protons** (particles with a positive electrical charge, p) and **neutrons** (neutral particles, n).
  [Exception: H nucleus has no neutrons.]
- Shells of **electrons** (particles with negative charge) surround the nucleus. Neutrons and protons are approx. 1800 times heavier than electrons.
- In its elemental ("neutral") state, an atom has **equal numbers of protons and electrons**.
- The **atomic number** of an element is the number of protons in the nucleus. It determines the chemical nature of the element.
- The **atomic mass** of an element is (approximately) the sum of the masses of protons, neutrons, and electrons present.



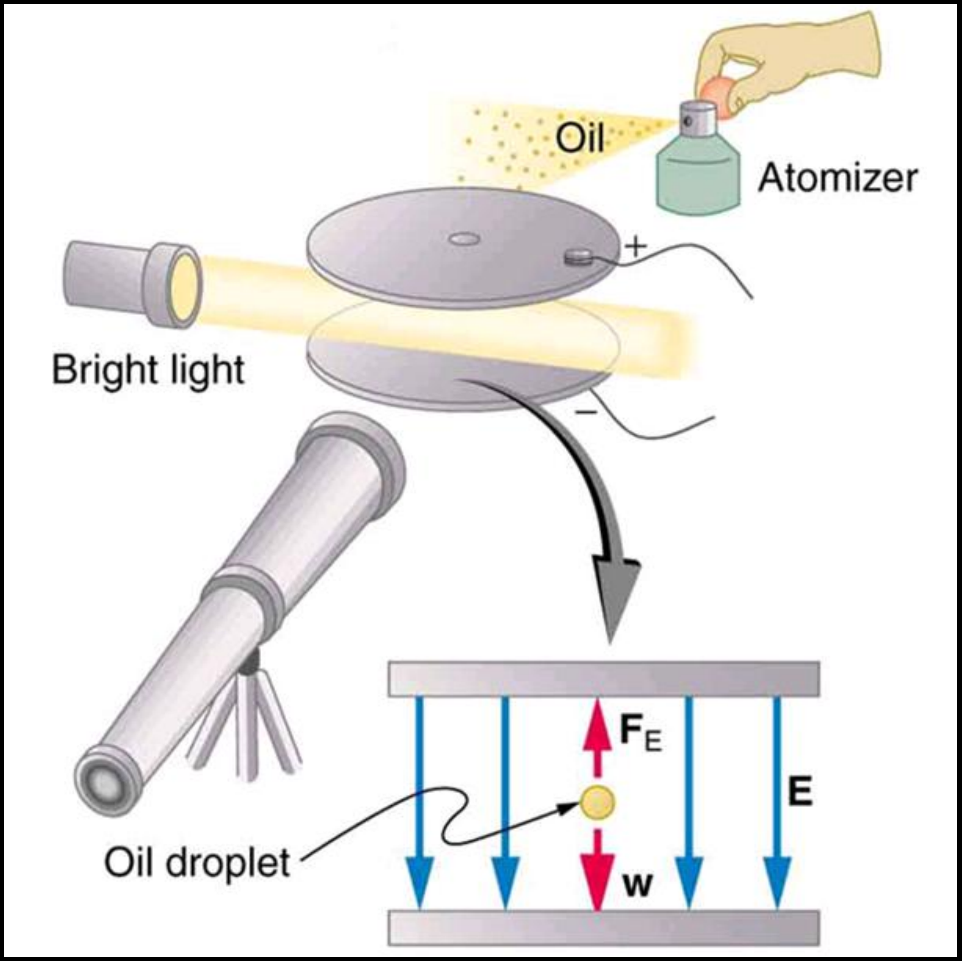


Atom = Nucleus (n, p) + Electrons



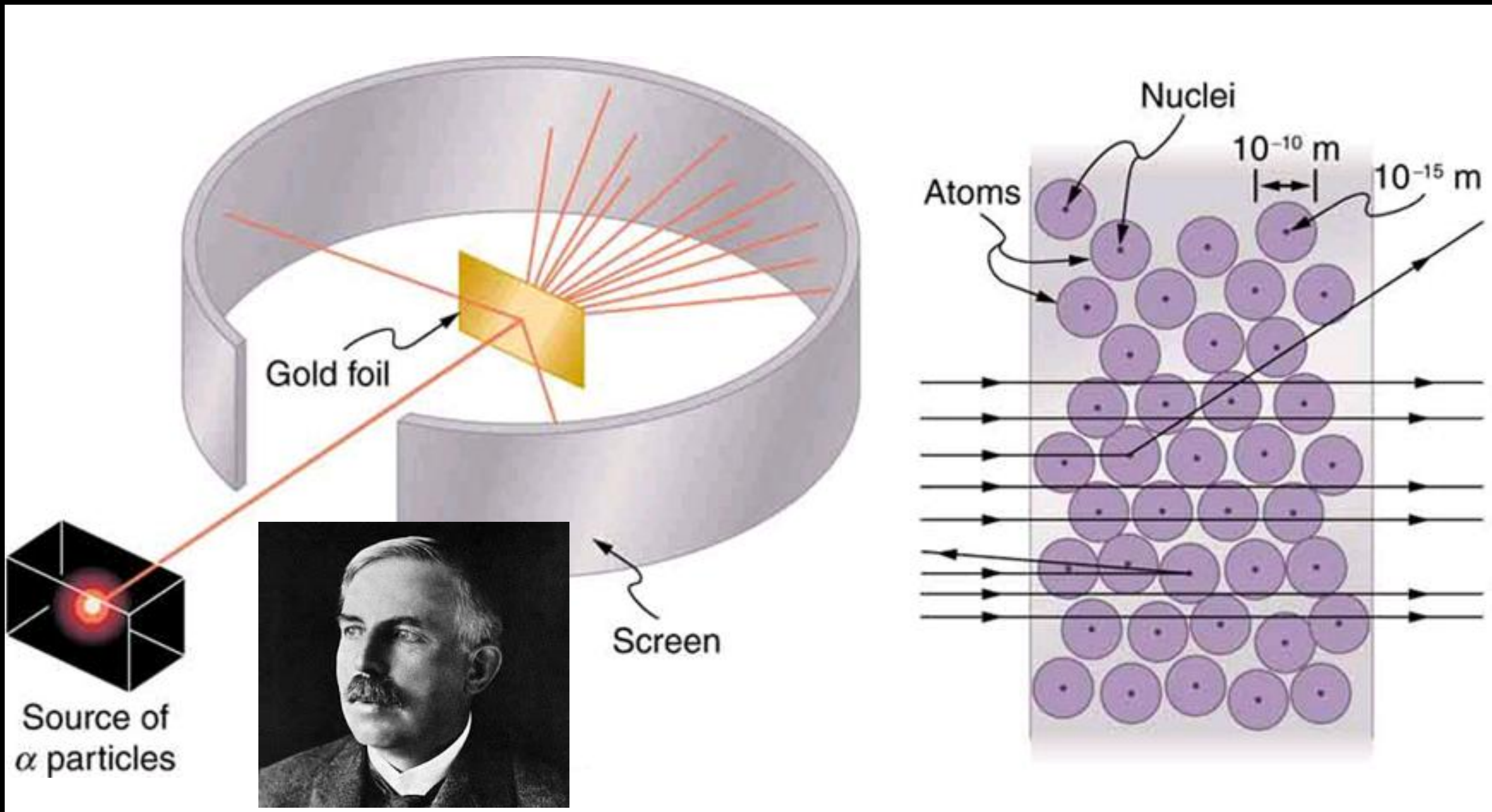


Discovery of the Electron (J. J. Thomson)



Charge of the Electron (R. Millikan)

Lecture 1 – **Atoms** – Introduction



Discovery of the Nucleus (E. Rutherford)

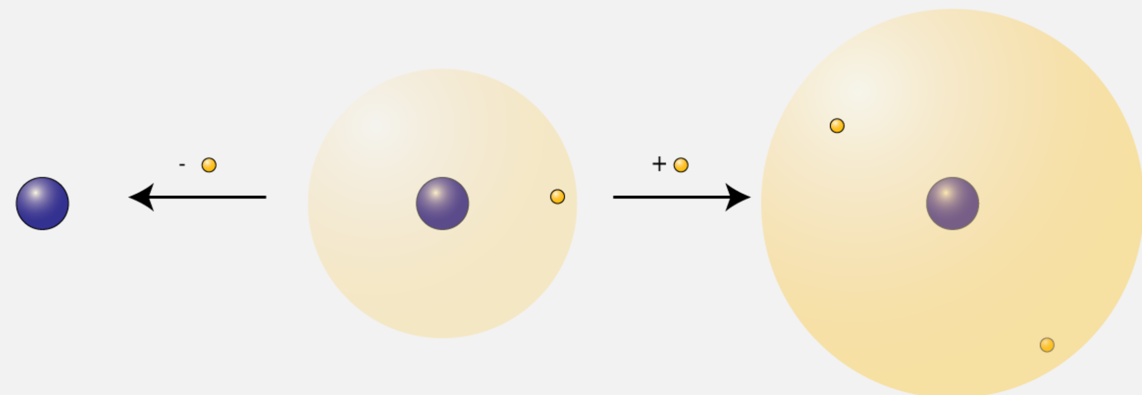
Lecture 1 – Atoms – Introduction

Atoms can gain or lose **electrons** to become more stable. Such a charged atom is called an **ion**.

- An atom that gains electrons becomes negatively charged and is an **anion**; an atom that loses electrons becomes positively charged and is a **cation**.

Atoms do not ordinarily gain or lose **protons** of the nucleus; note that this would change them into a **different element**. However, this can be enforced by nuclear reactions (also possible for **neutrons**).

Lecture 1 – Atoms – Introduction



No. of protons	1	1	1
No. of electrons	0	1	2
Charge	+1	0	-1
Notation	H^+	H	H^-
Classification	cation	neutral (not an ion)	anion

Ion = # Protons + #´ Electrons, where # ≠ #´

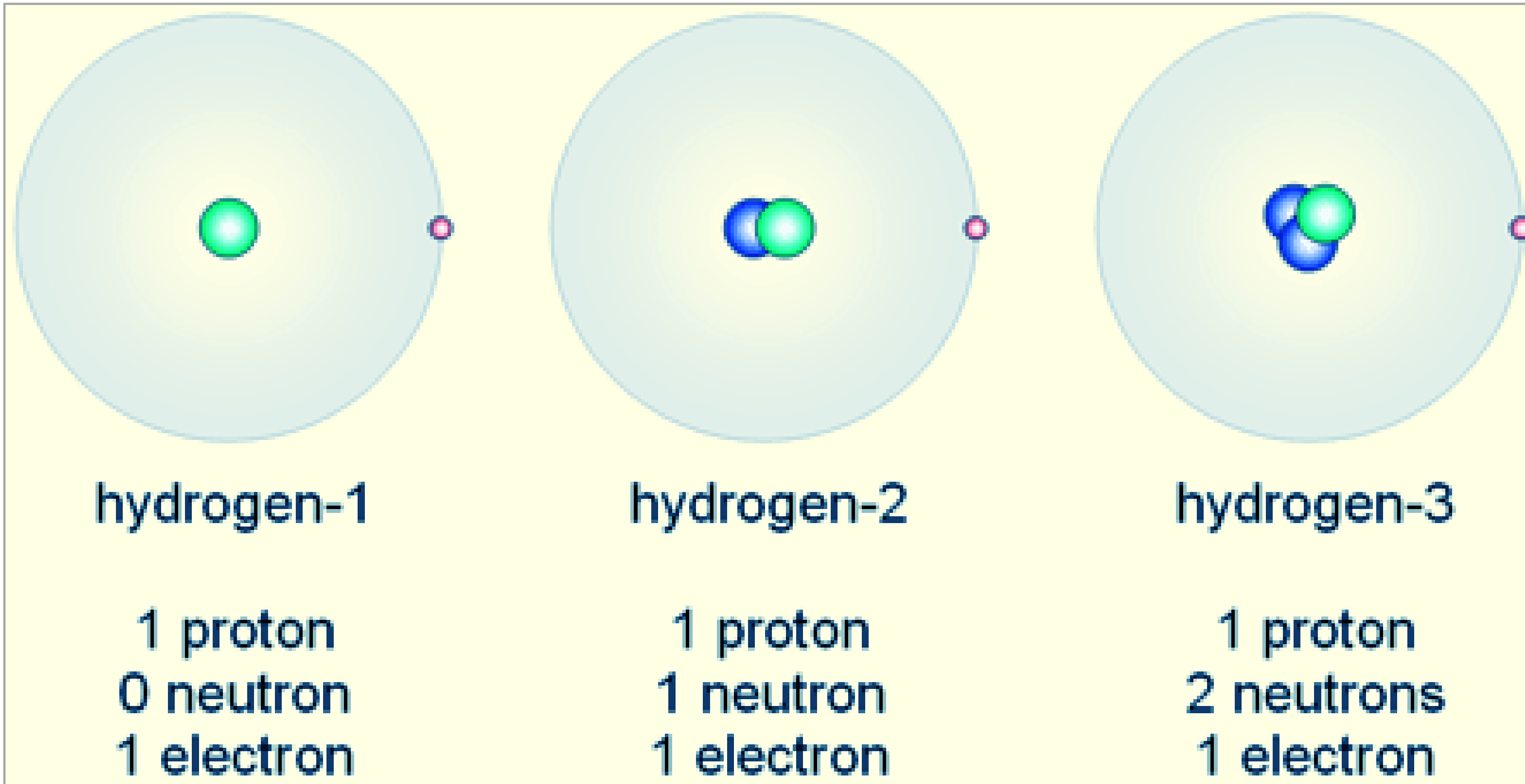
Lecture 1 – Atoms – Introduction

The **number of neutrons** in the nucleus can vary over a narrow range for an element.

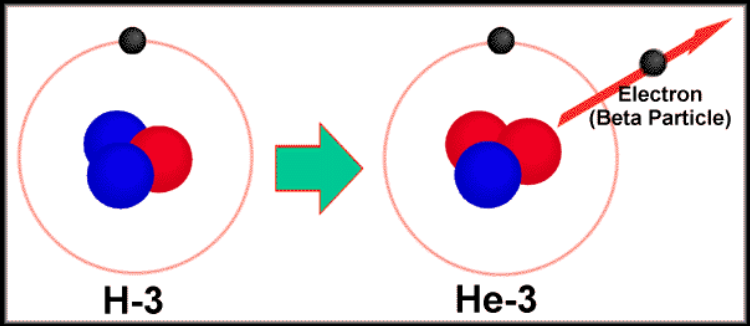
- The different forms have identical chemical properties but slightly different masses. They are **isotopes**. Some are stable, but others are unstable (**radioactive isotopes**).
- The different isotopes of an element are indicated by placing a superscript before the symbol, where the superscript is the sum of the protons and neutrons.

Example:

^{1}H, ^{2}H, and ^{3}H are the three isotopes of hydrogen, the first being by far the most common. ^{3}H is not stable but "radioactive":
it decays into ^{3}He, an electron and an anti-neutrino (→ more later)



Isotopes = Atoms with equal # p, different # n



Radioluminescence

Lecture 1 – **Atoms** – Introduction

The number of **electrons** in the outer shell of an element largely determines how it behaves chemically.

- Atoms with the same number of electrons in the outer shell show many similarities. This enables the construction of a **periodic table of the elements**.

→ Why this is so, will be the subject of this lecture!

Lecture 1 – Atoms – Introduction

JÜLICH FORSCHUNGSZENTRUM

Key

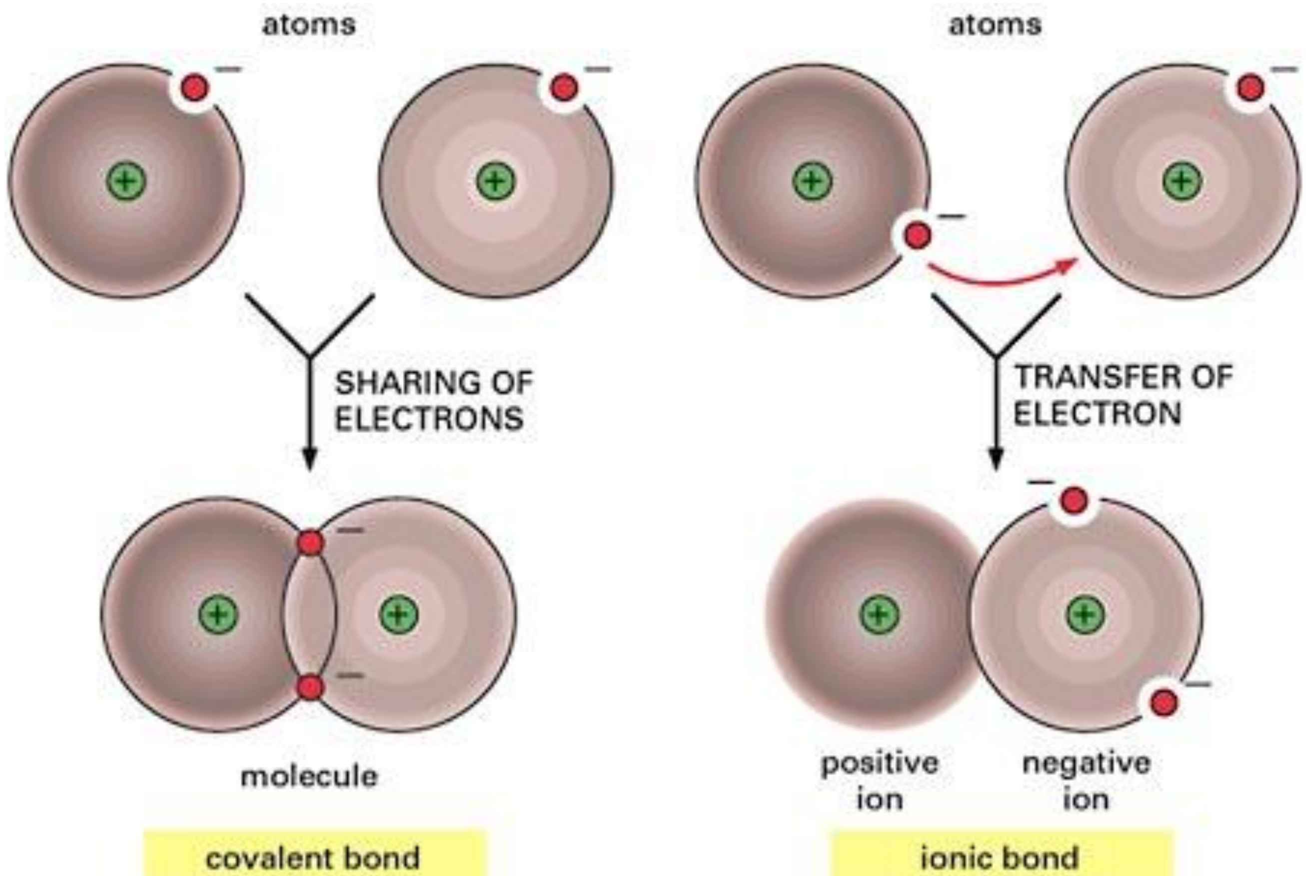
Atomic #
Symbol
Exact Name

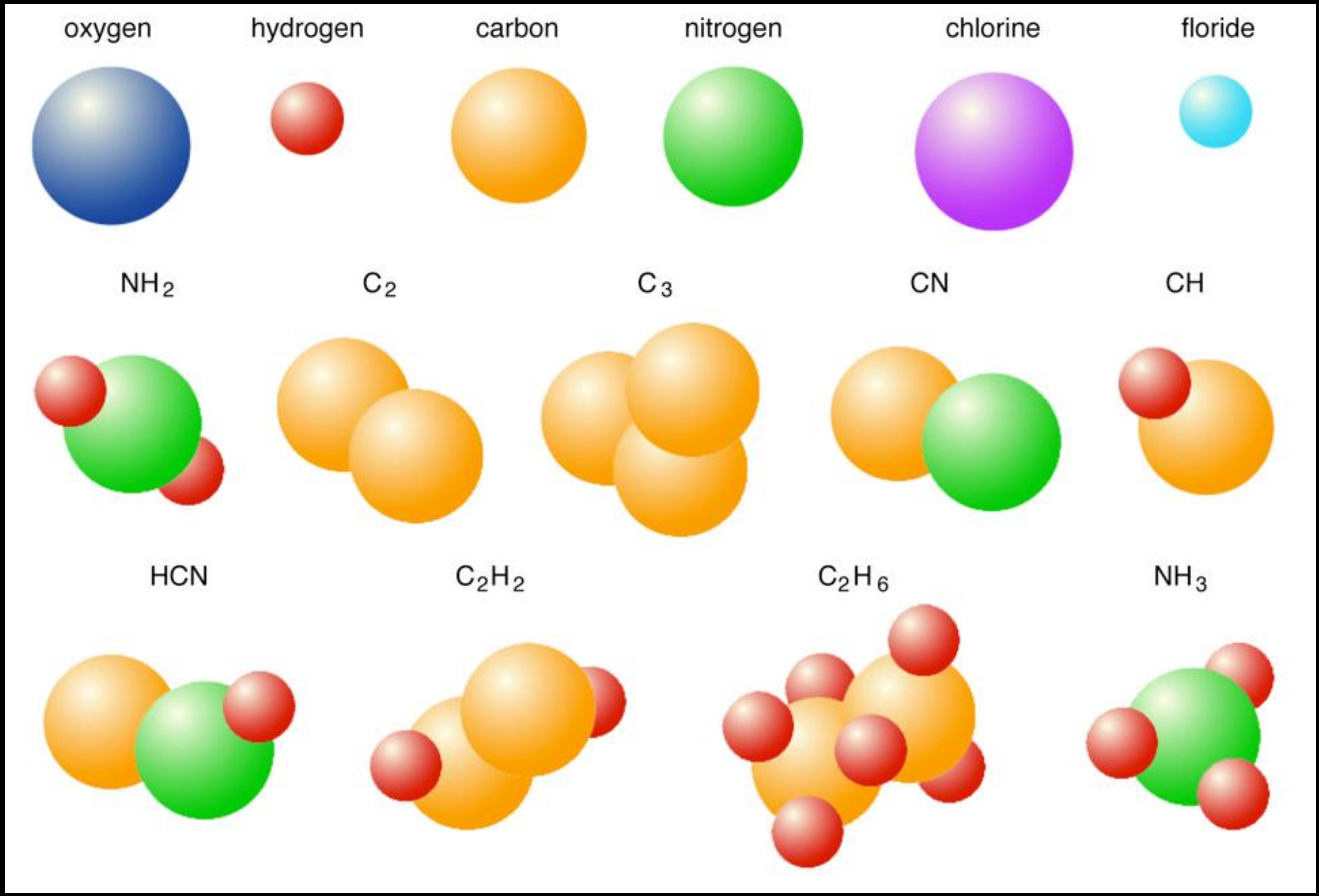
1 H Hydrogen																		2 He Helium
3 Li Lithium	4 Be Beryllium													5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon
11 Na Sodium	12 Mg Magnesium													13 Al Aluminum	14 Si Silicon	15 P Phosphorus	16 S Sulfur	17 Cl Chlorine	18 Ar Argon
19 K Potassium	20 Ca Calcium		21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton
37 Rb Rubidium	38 Sr Strontium		39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon
55 Cs Cesium	56 Ba Barium	*	71 Lu Lutetium	72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium	77 Ir Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Tl Thallium	82 Pb Lead	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon
87 Fr Francium	88 Ra Radium	**	103 Lr Lawrencium	104 Rf Rutherfordium	105 Db Dubnium	106 Sg Seaborgium	107 Bh Bohrium	108 Hs Hassium	109 Mt Meitnerium	110 Ds Darmstadtium	111 Rg Roentgenium	112 Cn Copernicium		114 Fl Flerovium		116 Lv Livermorium		

*	57 La Lanthanum	58 Ce Cerium	59 Pr Praseodymium	60 Nd Neodymium	61 Pm Promethium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dysprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium
**	89 Ac Actinium	90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium	95 Am Americium	96 Cm Curium	97 Bk Berkelium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendelevium	102 No Nobelium

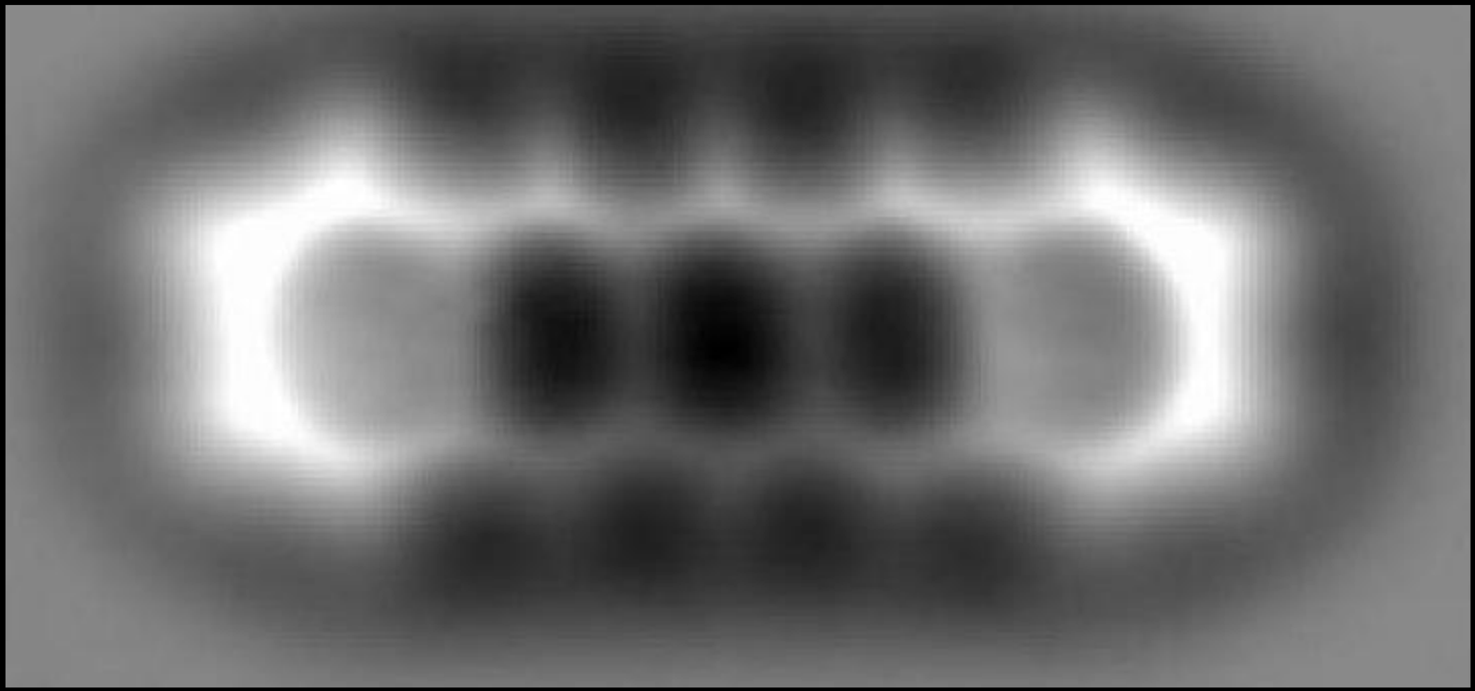
Lecture 1 – Atoms – Introduction

Atoms join together by means of **bonds** to form **molecules**.





Molecules = Combinations of Atoms

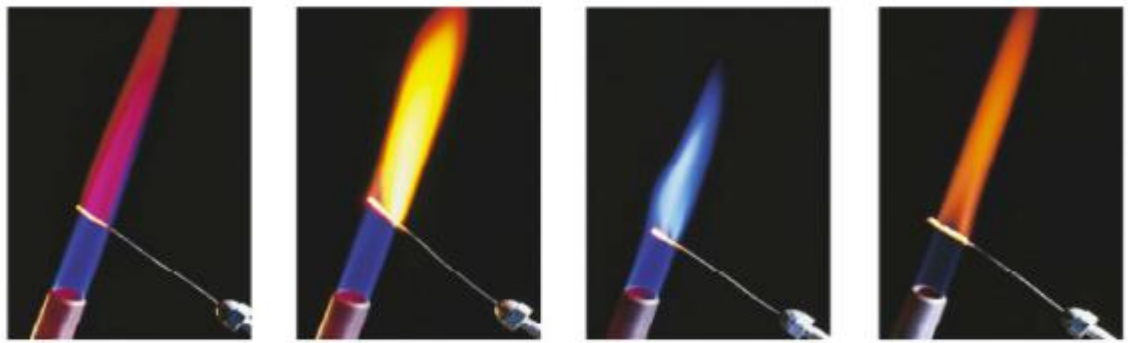


A pentacene molecule comprised of 22 carbon atoms and 14 hydrogen atoms observed with an atomic force microscope

A Picture of Atomic Bonds

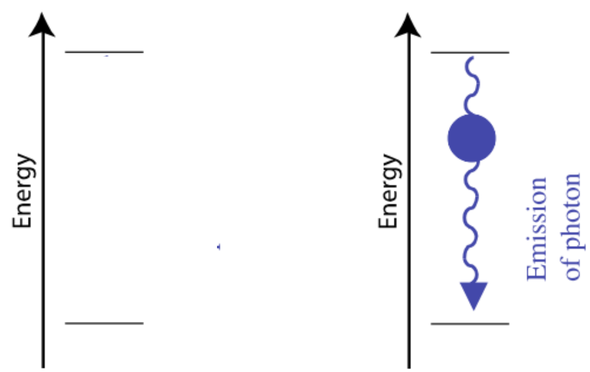
Lecture 1 – Atoms – Light Emission

When we put a sample of an element into a flame, it will shine in a color; examples:



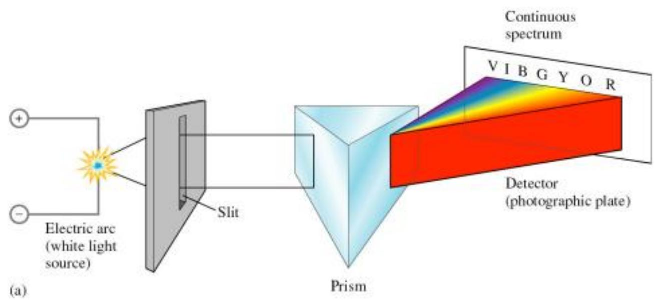
Li **Na** **K** **Ca**

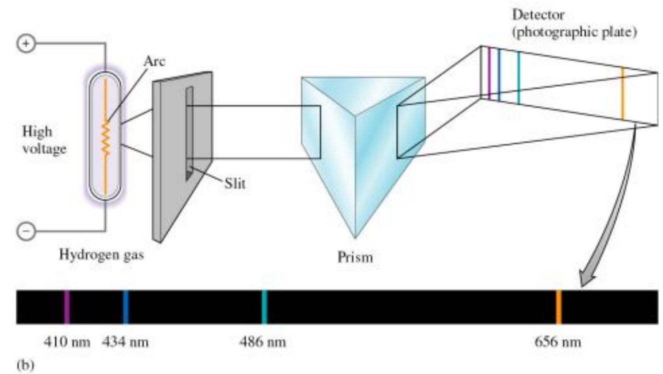
The atoms first become **excited**; when the relax, they emit, e.g., visible light, the color of which depends on the element:



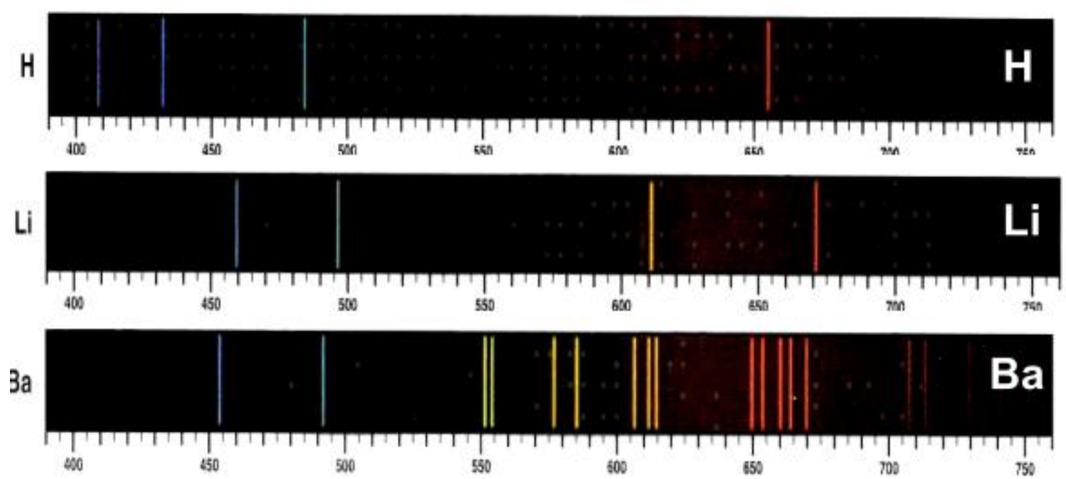
Lecture 1 – Atoms – Light Emission

When the light emitted from a excited atoms is passed through a prism, discrete bands of color at **specific wavelengths** are observed:



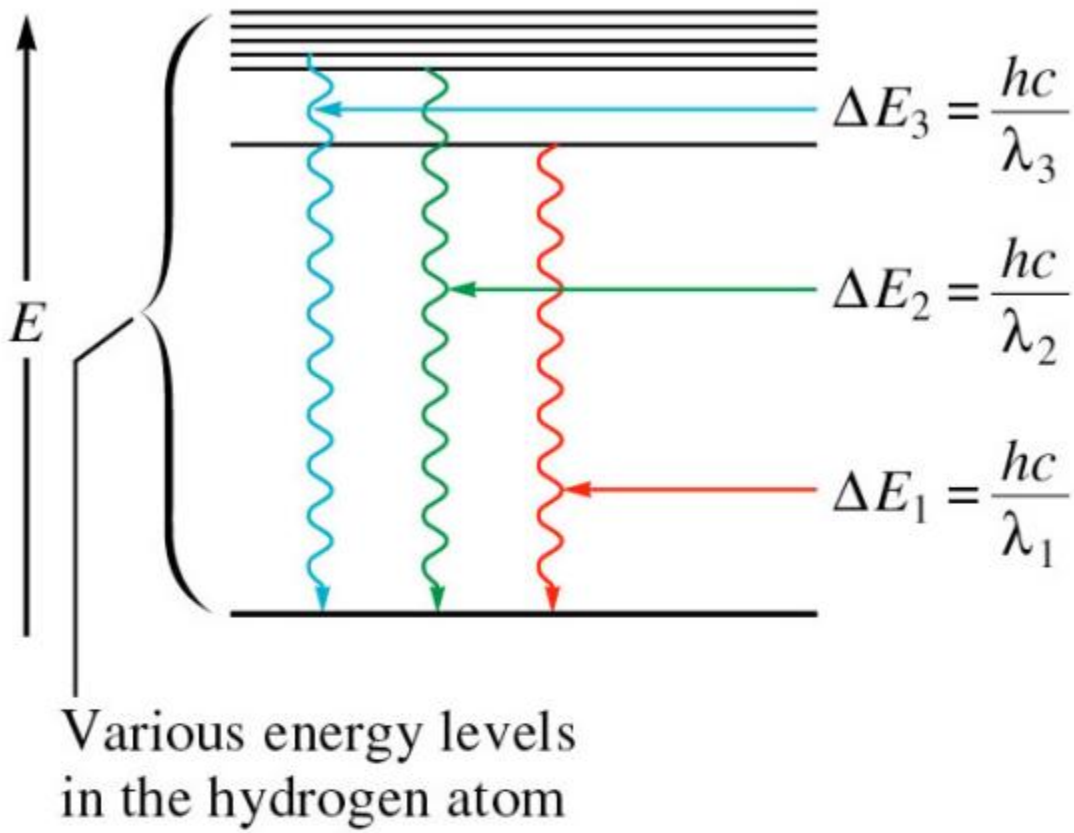


Examples:



Lecture 1 – Atoms – Light Emission

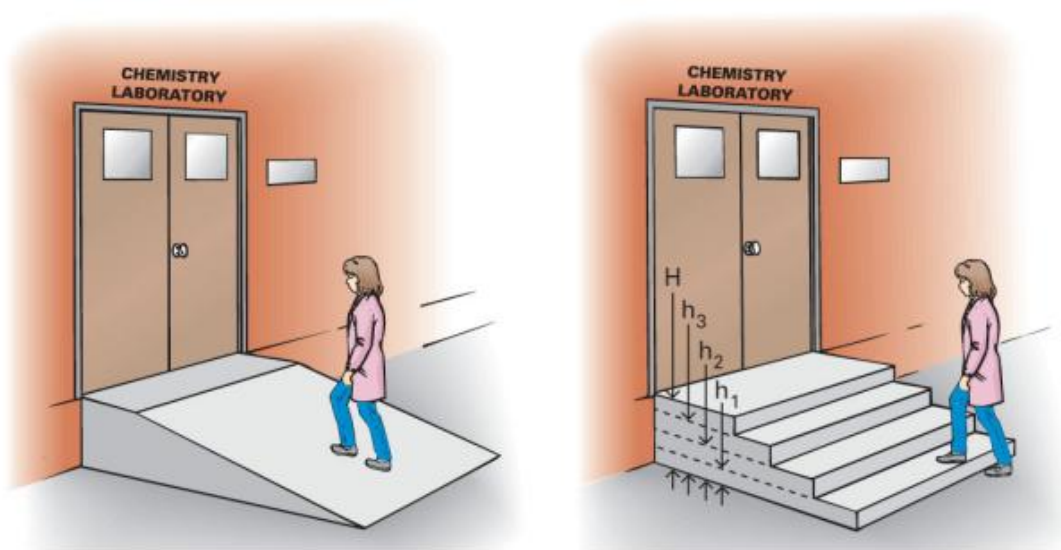
The light emission spectrum of hydrogen (and other atoms) can be used to determine the **excitation energy levels** in the atom:



Lecture 1 – Atoms – Light Emission

The atomic energy levels are **quantized**, i.e. the energies available to an atom do not form a continuum, but have discrete values:

Energy Quantization

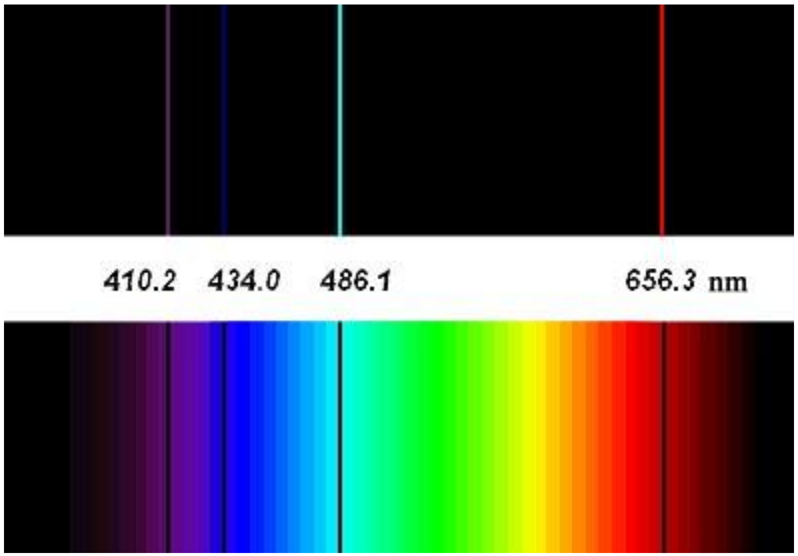


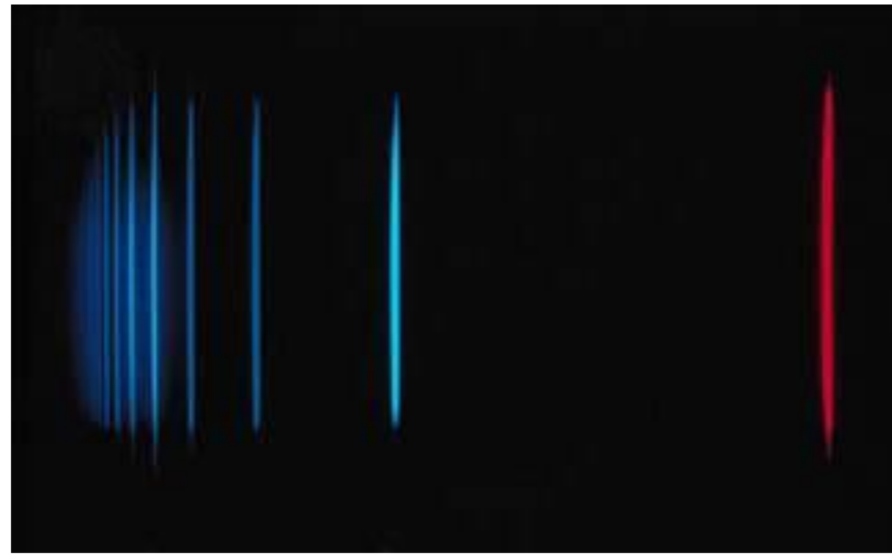
The student can stop at any point on the ramp. Her distance from the ground changes continuously.

The student can stop only at certain points on a flight of stairs. Her distance from the ground is ***quantized***.

Lecture 1 – **Atoms** – Light Emission

The visible part of the light emitted from (or absorbed by) hydrogen was first investigated by **Johann Jakob Balmer** (1885):



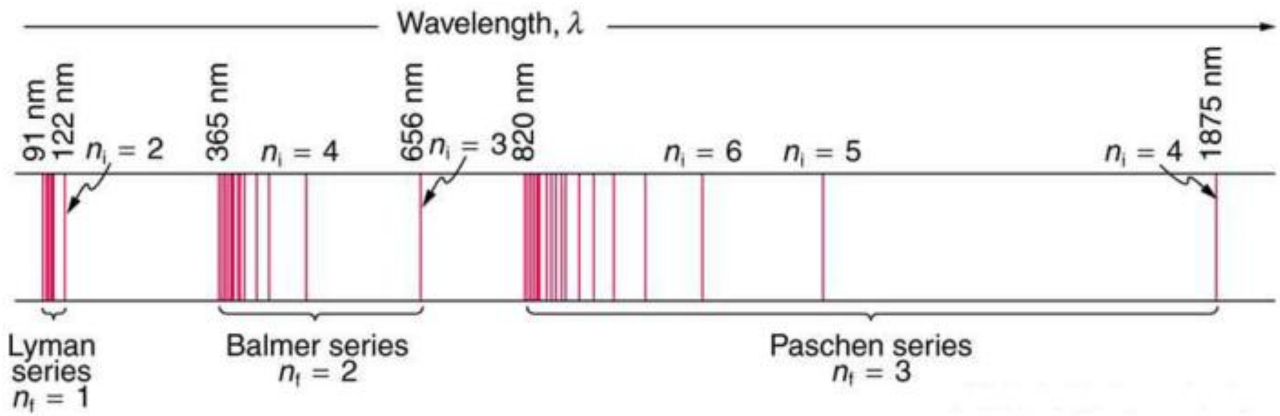


He found the following **empirical relation** for the wavelengths λ of the spectral lines:

$$\lambda = A\left(\frac{n^2}{n^2-4}\right) = A\left(\frac{n^2}{n^2-2^2}\right).$$

Lecture 1 – Atoms – Light Emission

Subsequently, other spectral lines were found both in the UV (smaller wavelengths) and in the IR (larger wavelengths):

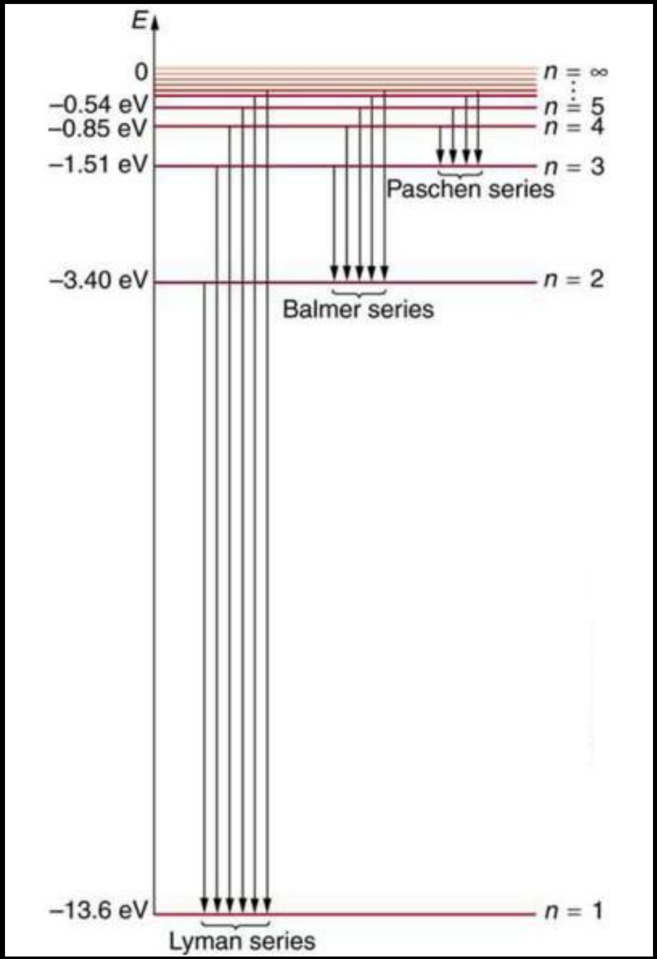


In 1888, **Johannes Rydberg** presented a formula to describe all of them:

$$\frac{1}{\lambda_{\mathrm{vac}}} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

Here, n_1 (= 1, 2, 3, …) and n_2 are integers such that $n_1 < n_2$ (= n_1 + 1, …); R is the so-called Rydberg-constant

$$R = 1.097\times10^7\,/\,\mathrm{m}\ (\mathrm{or\ m}^{-1}).$$



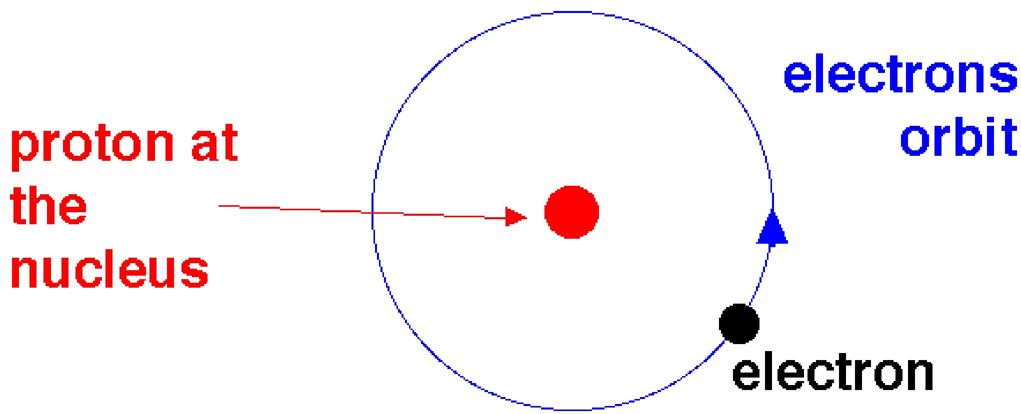
"Series"

$n_1 = 1$	$n_2 = 2, 3, 4, 5, 6, 7, \ldots$	Lyman
$n_1 = 2$	$n_2 = 3, 4, 5, 6, 7, \ldots$	Balmer
$n_1 = 3$	$n_2 = 4, 5, 6, 7, \ldots$	Paschen
$n_1 = 4$	$n_2 = 5, 6, 7, \ldots$	Brackett
$n_1 = 5$	$n_2 = 6, 7, \ldots$	Pfund
$n_1 = 6$	$n_2 = 7, \ldots$	Humphreys
…		

The Spectral Lines of Hydrogen

Lecture 1 – Atoms – Bohr Model

The **Bohr model**, introduced by **Niels Bohr** in 1913, depicts the atom as small, positively charged nucleus surrounded by electrons that travel in circular orbits around the nucleus – similar in structure to the solar system, but with attraction provided by **electrostatic forces** rather than gravity.



The model's key success lay in **explaining the Rydberg formula** for the spectral emission lines of atomic hydrogen.

Key questions: (i) why does electron not “fall into” nucleus ?
(ii) why are only certain energies allowed ?

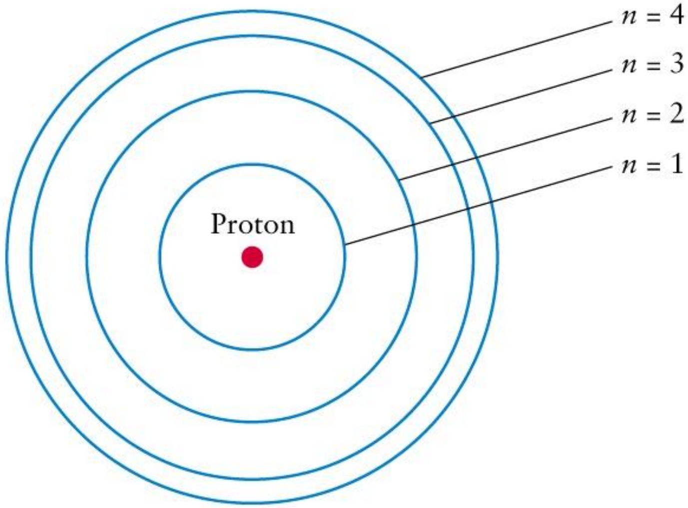
Lecture 1 – **Atoms** – Light Emission

Niels Bohr

Lecture 1 – **Atoms** – Bohr Model

N. Bohr proposed that electrons could only have certain *classical* motions:

- The electrons can only orbit in certain discrete distances from the nucleus.



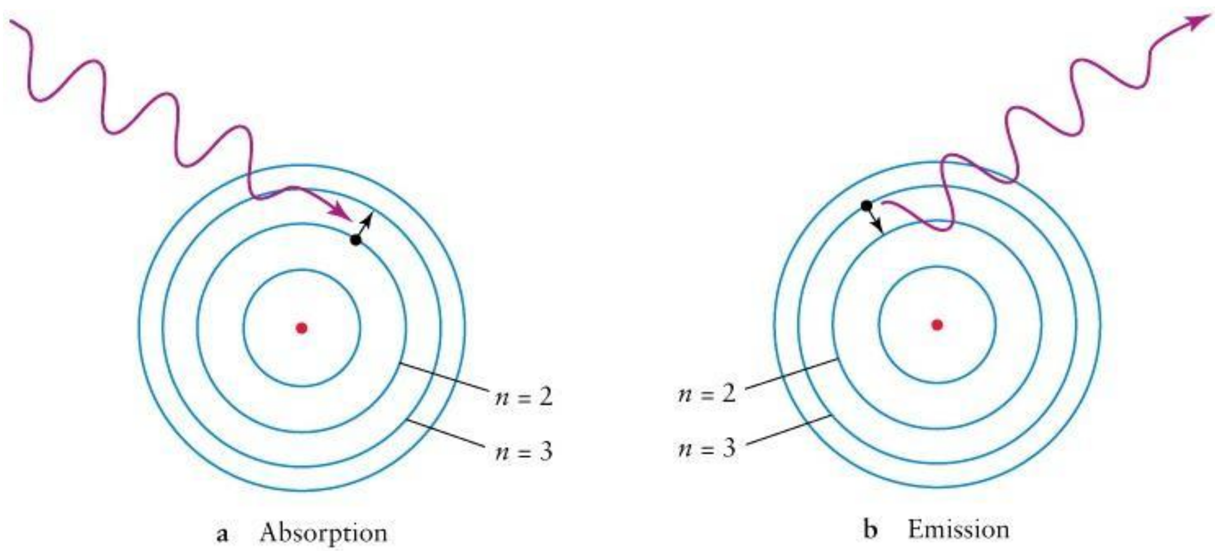
These orbits are associated with definite energies and are also called **energy shells** or **energy levels**. In these orbits, the electron's acceleration does not result in radiation and corresponding energy loss as required by classical electromagnetics.

Lecture 1 – **Atoms** – Bohr Model

N. Bohr proposed that electrons could only have certain *classical* motions:

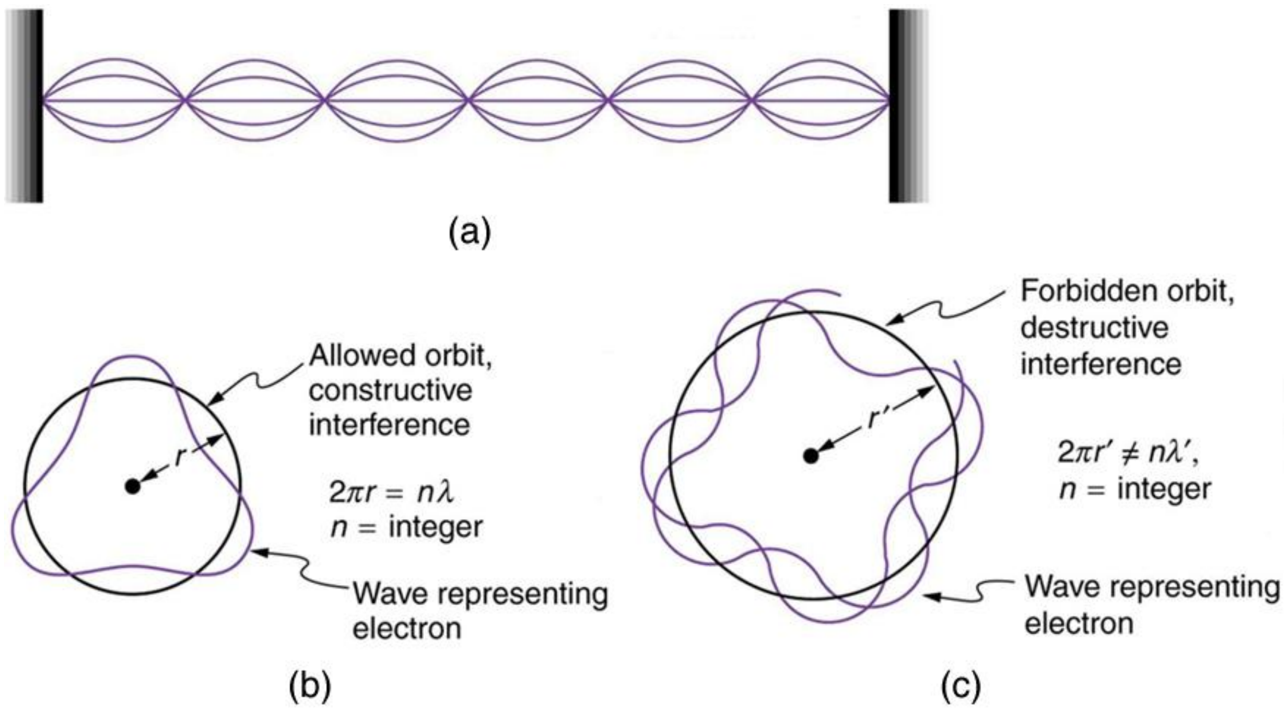
- Electrons can only **gain and lose energy** by jumping from one allowed orbit to another, absorbing or emitting electromagnetic radiation with a frequency ν determined by the energy difference of the levels according to the *Planck relation*:

$$\Delta E = E_2 - E_1 = h\nu$$



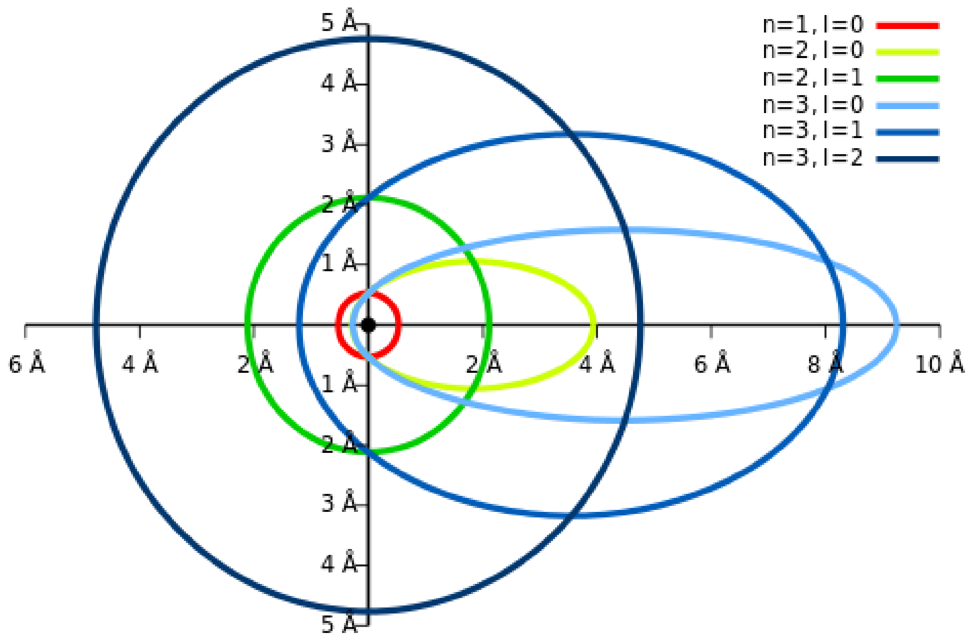
Lecture 1 – Atoms – Bohr Model

N. Bohr's final condition (the angular momentum is an integer multiple of $\hbar$) was reinterpreted in 1924 by **L. de Broglie** as a standing wave condition: the electron is described by a wave and a whole number of wavelengths must fit along the circumference of the electron's orbit:



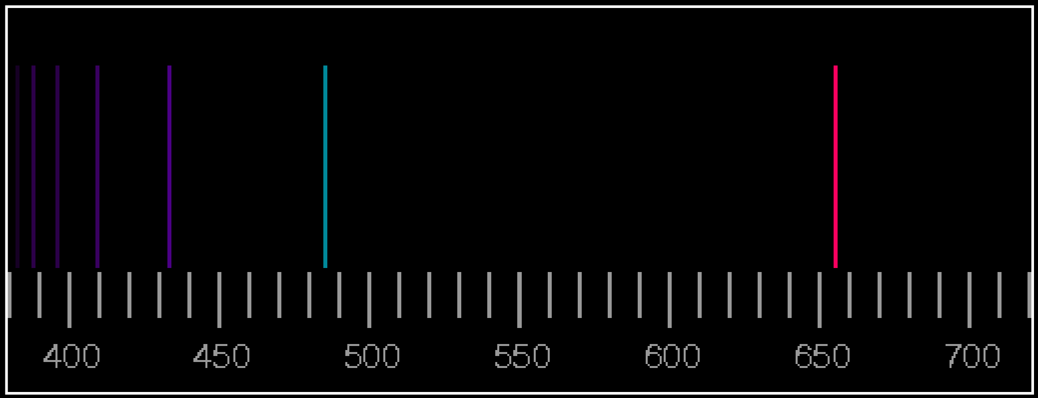
Lecture 1 – Atoms – Bohr Model

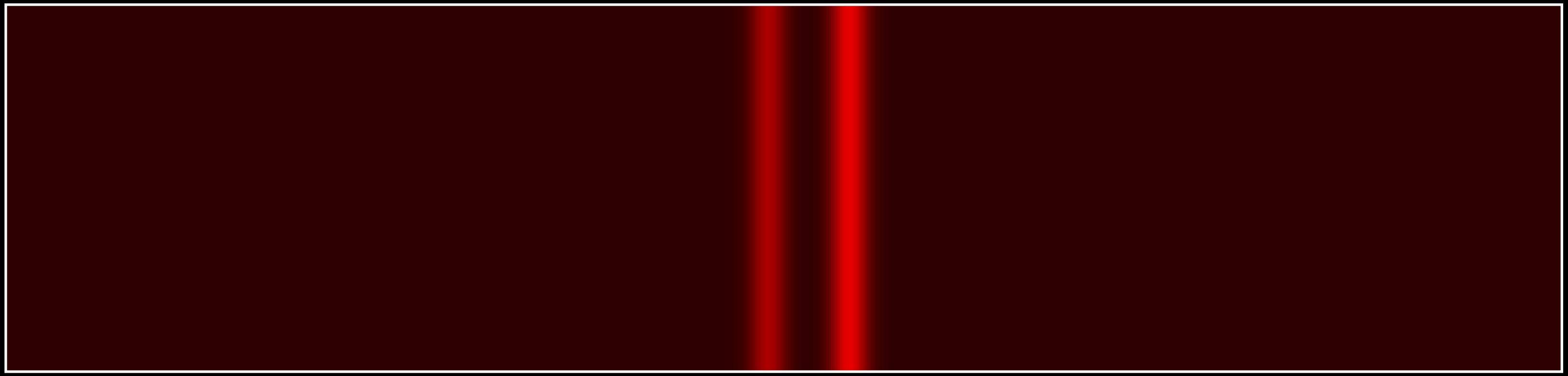
The **Bohr-Sommerfeld model** (1916) was a refinement, still based on classical mechanics: it assumes that electrons orbit the nucleus in ellipses (like planets …) and has two characteristic numbers (n, l):



Main avantage: it could explain the so-called **fine-structure** of the spectral lines, making use of relativistic corrections …

Lecture 1 – Atoms – Light Emission

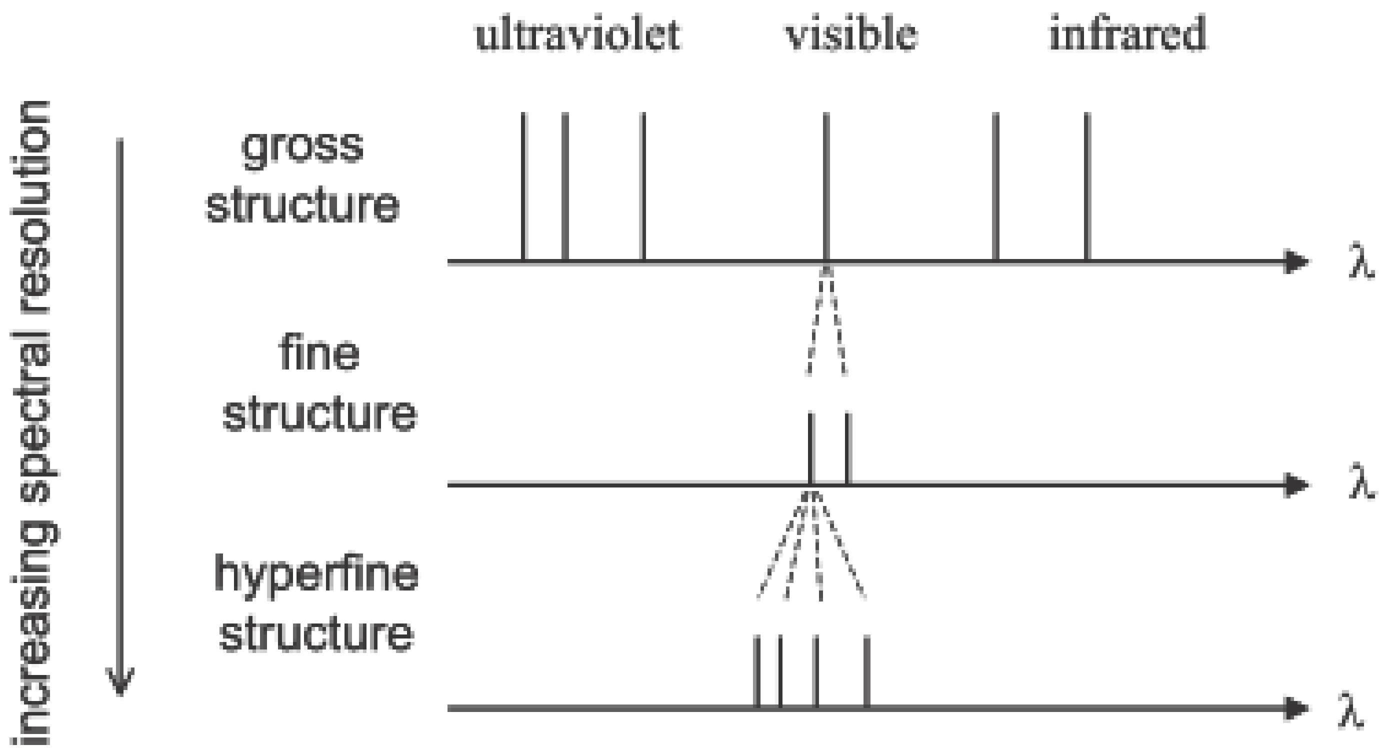




Fine structure of Balmer (H_α) line

Lecture 1 – Atoms – Bohr Model

Things turn out to be (much) **more complex** … **and interesting** !

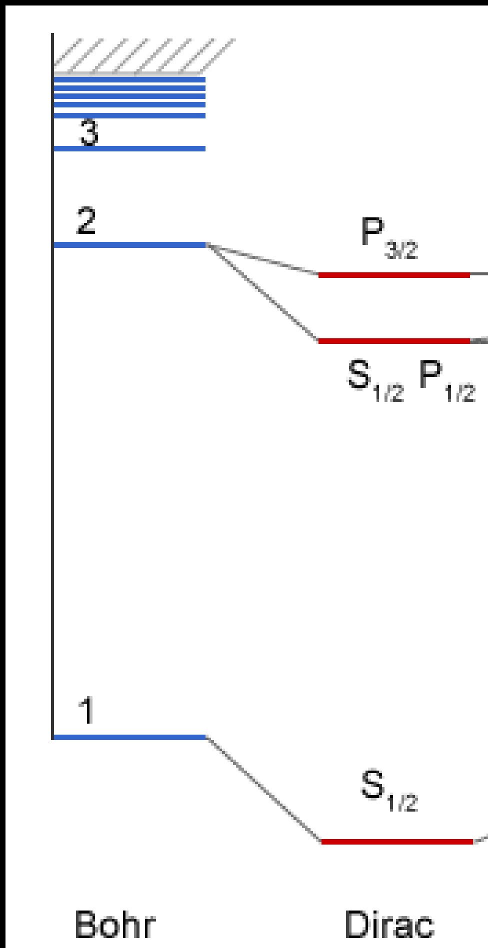


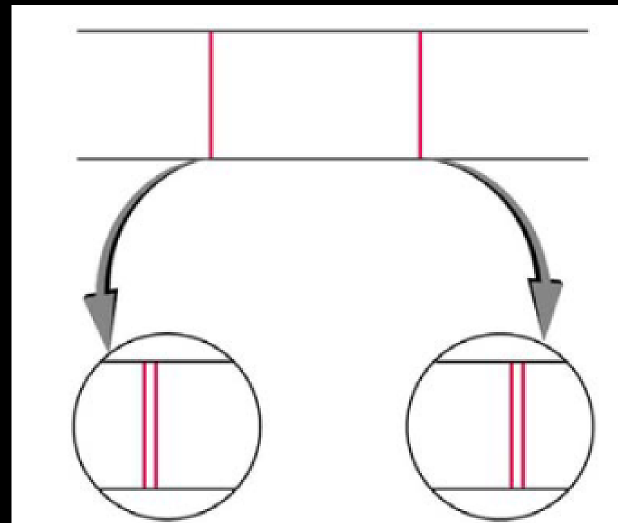
Lecture 1 – **Atoms** – Bohr Model

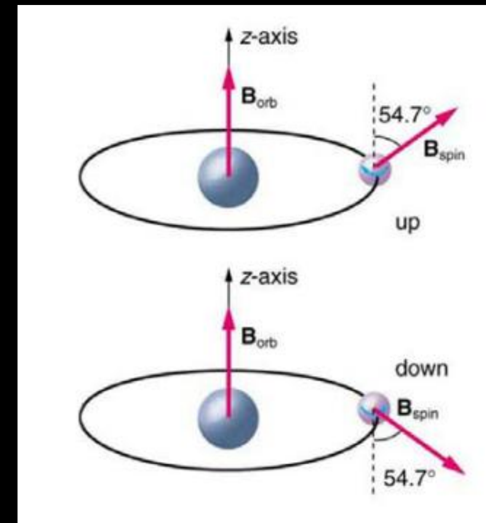
In order to fully understand the hydrogen atom, one needs (relativistic) **quantum mechanics** (which is beyond the scope of this lecture);

- The Bohr model does not always fully respect the "**Heisenberg Uncertainty Principle**", which states that the position of the electron and its momentum cannot be known with arbitrary precision simultaneously.
- The **electron** exhibits an internal characteristics called "**spin**", and an associated "spin magnetic moment", which provides two different states (energies) in any magnetic field.
- The same holds true for the **proton** (and **neutron**); all of them are called "**fermions**".
- The space, in which a hydrogen atom sits, is never empty, but it contains **particle-antiparticle pairs**, which interact, e.g., with the electron.

Lecture 1 – Atoms – QM Model



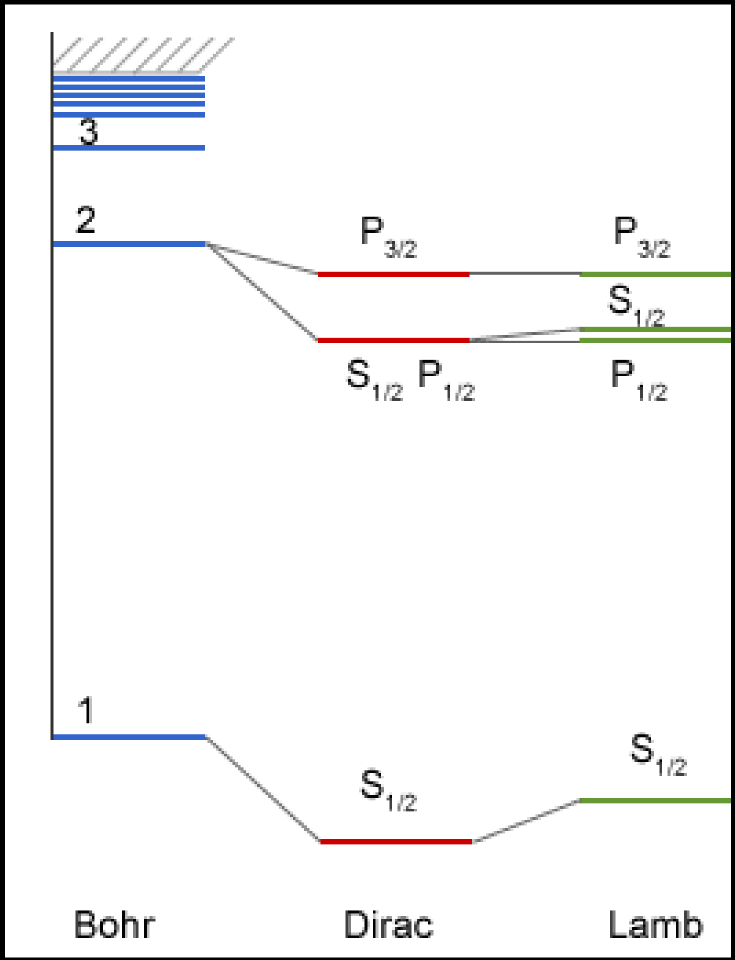


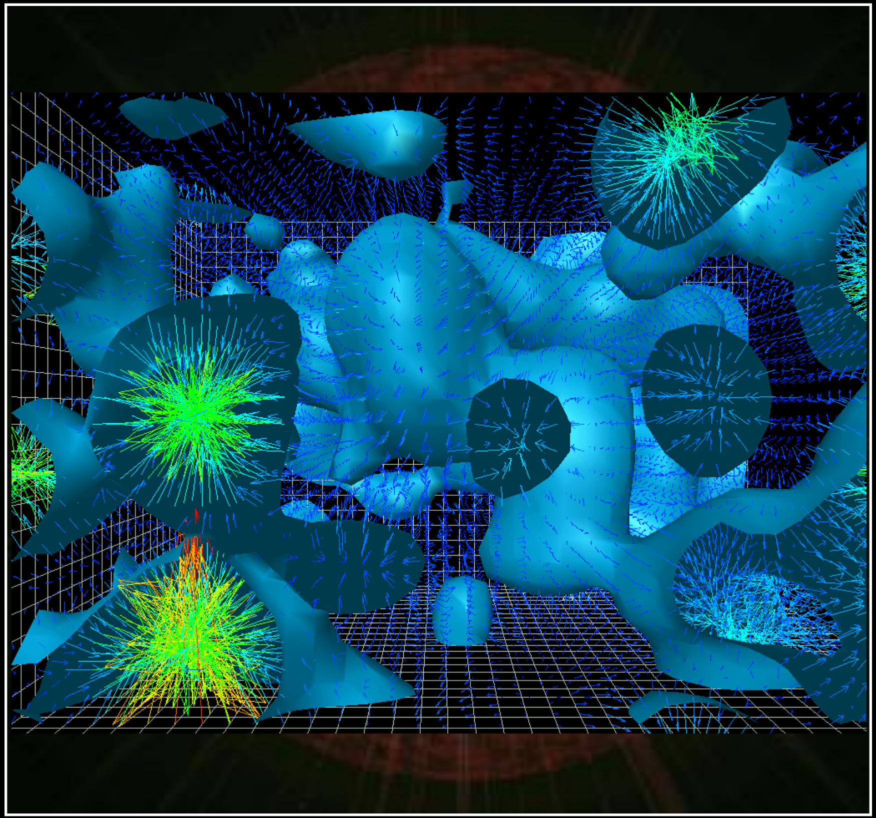


The intrinsic magnetic field of the electron due to its spin interacts with the magnetic field of the electron caused by its orbital motion (spin-orbit interaction):
→ spectral lines are split into two („doublets“).

Fine structure of hydrogen

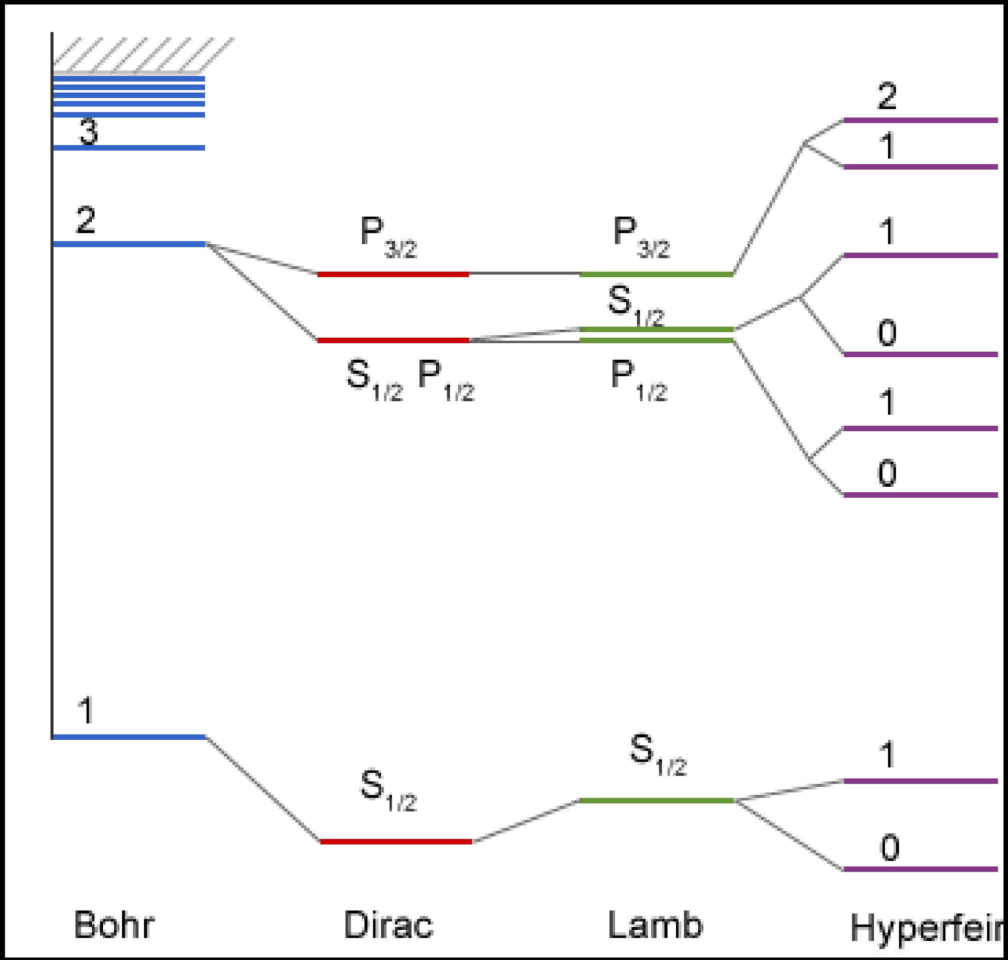
Lecture 1 – **Atoms** – QM Model





Interaction with the vacuum

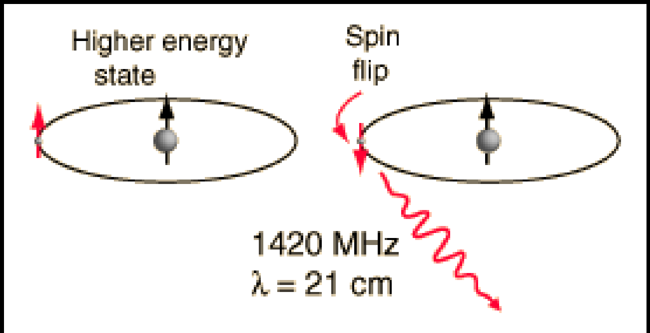
Lamb Shift → Quantum-Electrodynamics



The hyperfine splitting is due to the interaction of the magnetic field of the electron with the magnetic field of the proton (i.e. the nucleus) [Note: energy splitting is **not to scale**:

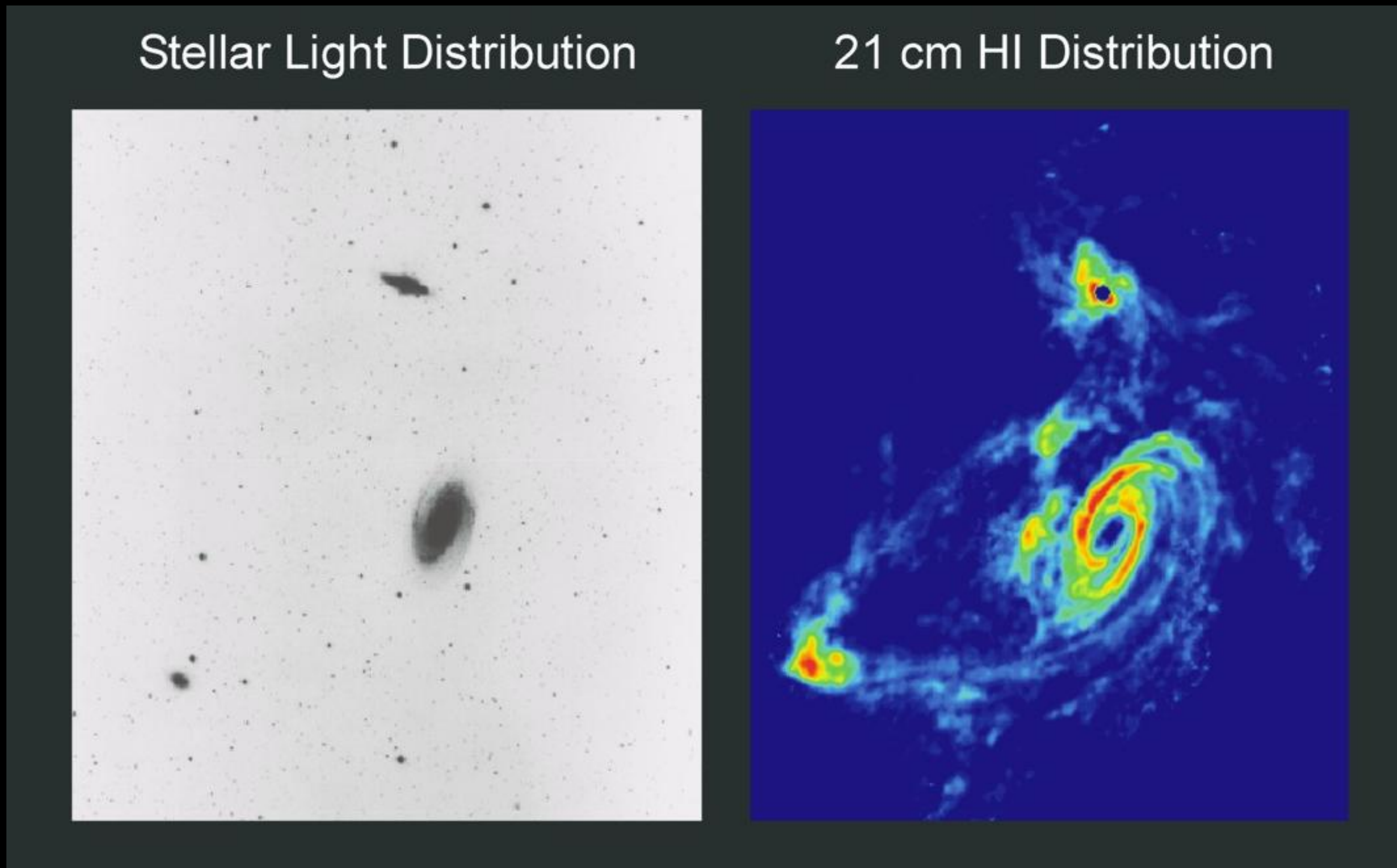
FS $\sim 10^{-4} – 10^{-5}$ eV

HFS $\sim 10^{-7} – 10^{-8}$ eV]



„Complete“ hydrogen spectrum

Lecture 1 – **Atoms** – Light Emission



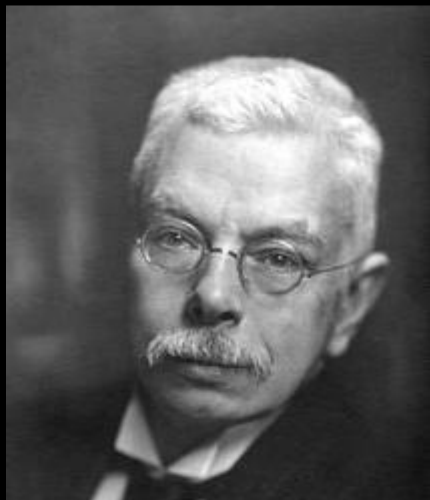
21 cm hydrogen line in the universe

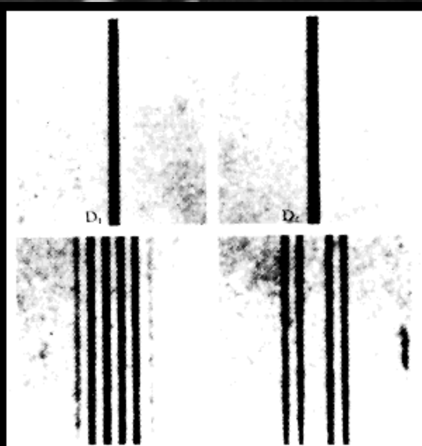
Lecture 1 – **Atoms** – QM Model

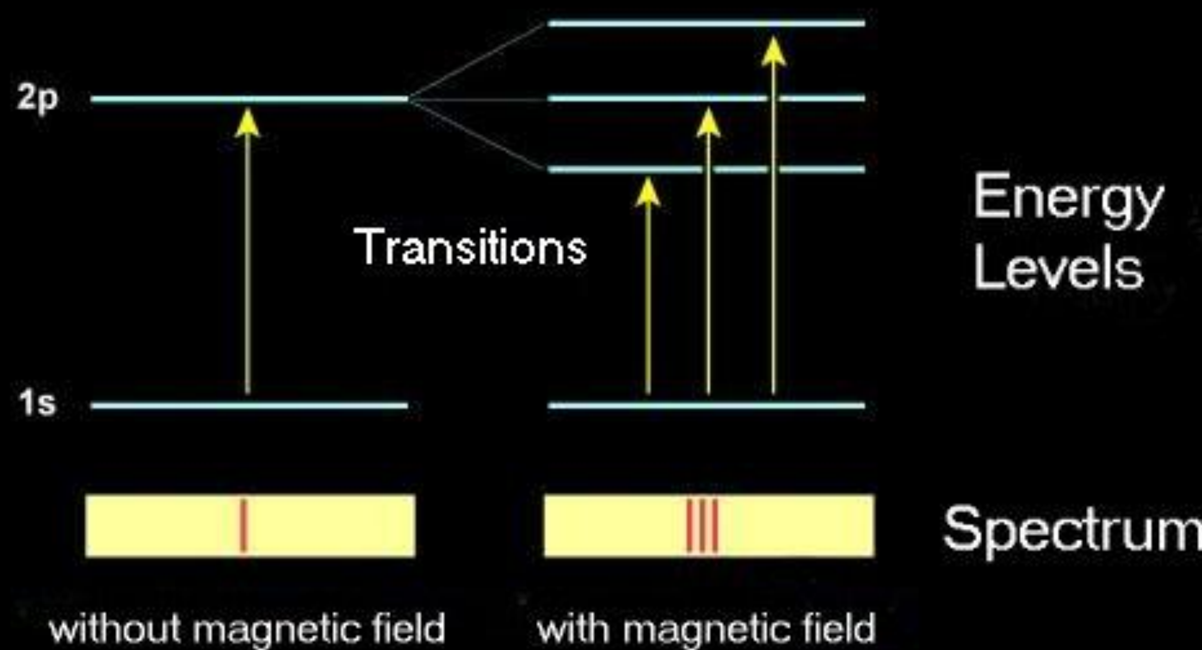
Hydrogen in an **external magnetic** or **electric fields**: new effects

Applied field	Field strength	Effect
Magnetic	weak strong	Zeeman Paschen-Back
Electric	all	Stark

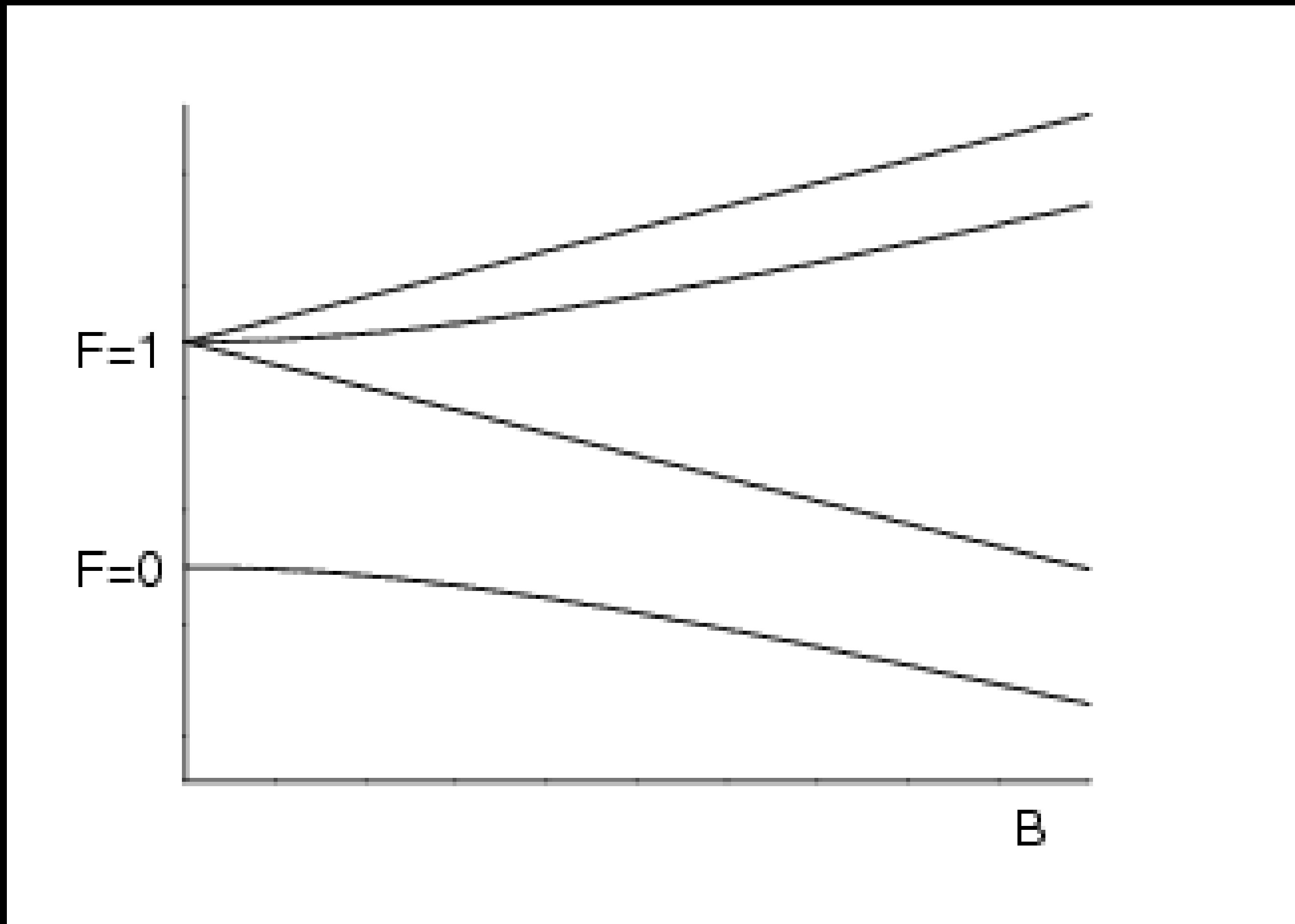
E.g.: When an external magnetic field is applied, sharp spectral lines of hydrogen split into multiple closely spaced lines. First observed by **Pieter Zeeman** in 1896, this splitting is attributed to the interaction between the external magnetic field and the magnetic field associated with the orbital angular momentum of the electron.





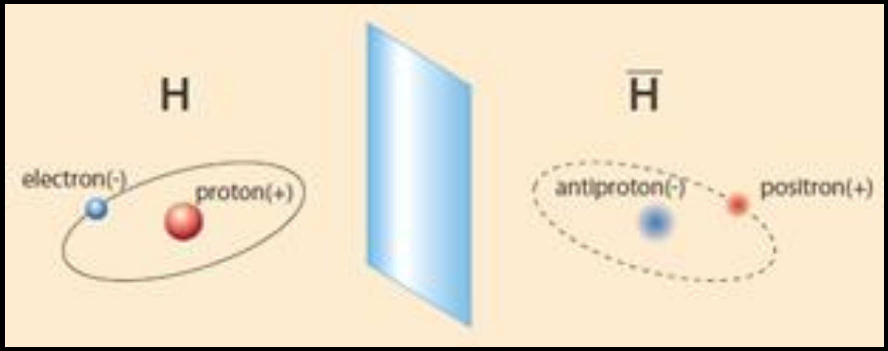


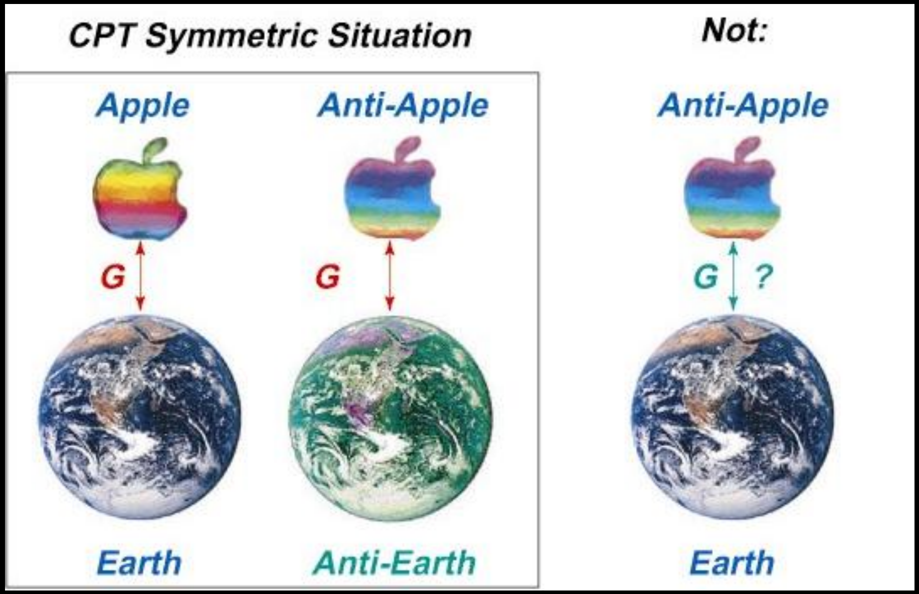
Zeeman splitting (B-field)

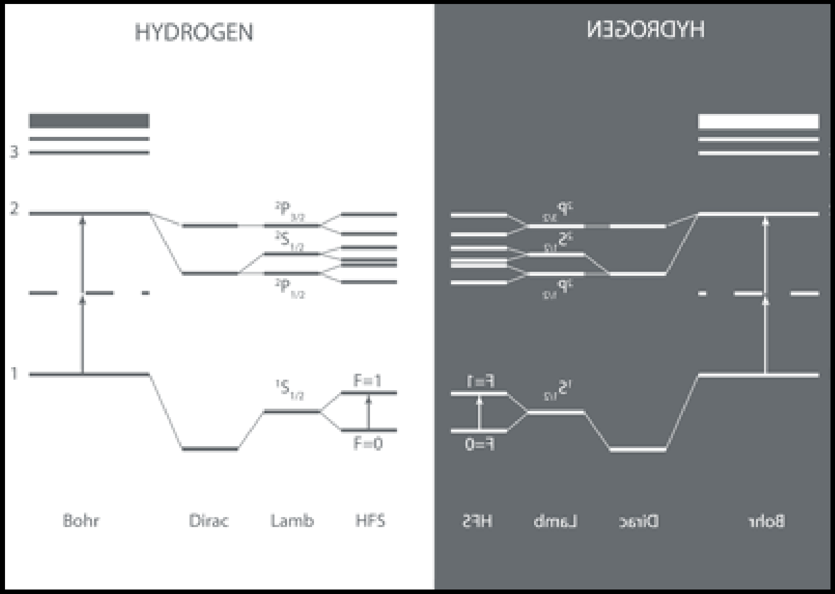


Breit-Rabi diagram

Lecture 1 – **Atoms** – QM Model





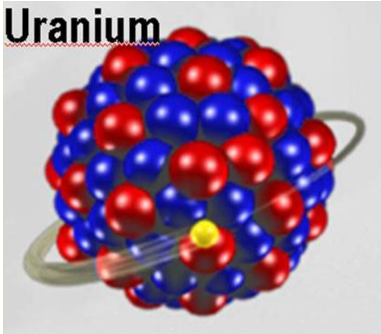


Hydrogen and Anti-Hydrogen

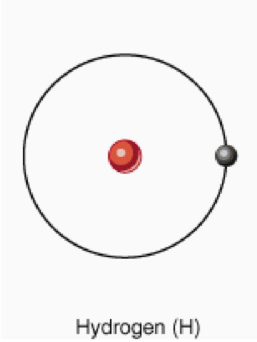
Lecture 1 – Atoms – QM Model

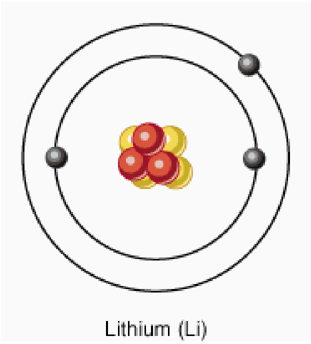
Atoms with **more than one electron** … will be even more complex and complicated; the most simple cases are:

- atoms, which have lost all but one electron (“**hydrogen-like ions**”) e.g.:

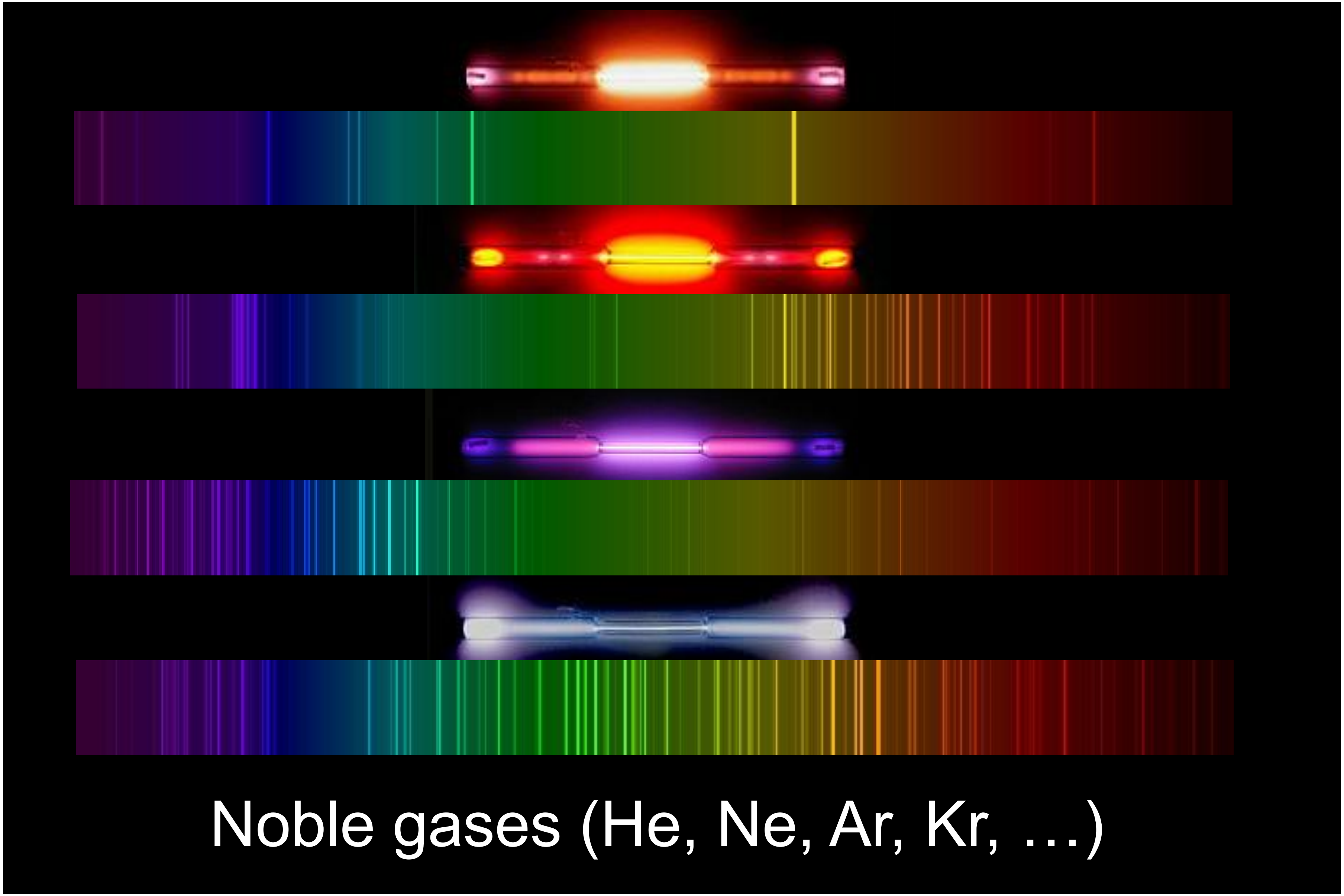


- atoms, which have only one electron in the outermost electron shell (“**alkali atoms**”) e.g.;





Lecture 1 – Atoms – Light Emission



Lecture 1 – Atoms – Light Emission

Aurora Borealis (Northern Light)

Lecture 1 – **Atoms** – QM Model

Nature´s plan to build the (chemical) elements:

The most important constraint is the "Pauli Exclusion Principle" after **Wolfgang Pauli**:

No two "fermions" can exists in identical quantum states.

Applied to atoms, this principle has most profound consequences:

No two **electrons** in an atom can have identical quantum numbers.

There are the following **four quantum numbers**:

Table 30.1 Atomic Quantum Numbers

Name	Symbol	Allowed values
Principal quantum number	n	$1, 2, 3, \ldots$
Angular momentum	l	$0, 1, 2, \ldots n-1$
Angular momentum projection	m_l	$-l, -l+1, \ldots, -1, 0, 1, \ldots, l-1, l$ (or $0, \pm 1, \pm 2, \ldots, \pm l$)
Spin[1]	s	$1/2$(electrons)
Spin projection	m_s	$-1/2, +1/2$

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Principal Quantum Number, n = 1

n	ℓ	m_ℓ	m_s
1	0	0	+ 1/2
1	0	0	– 1/2

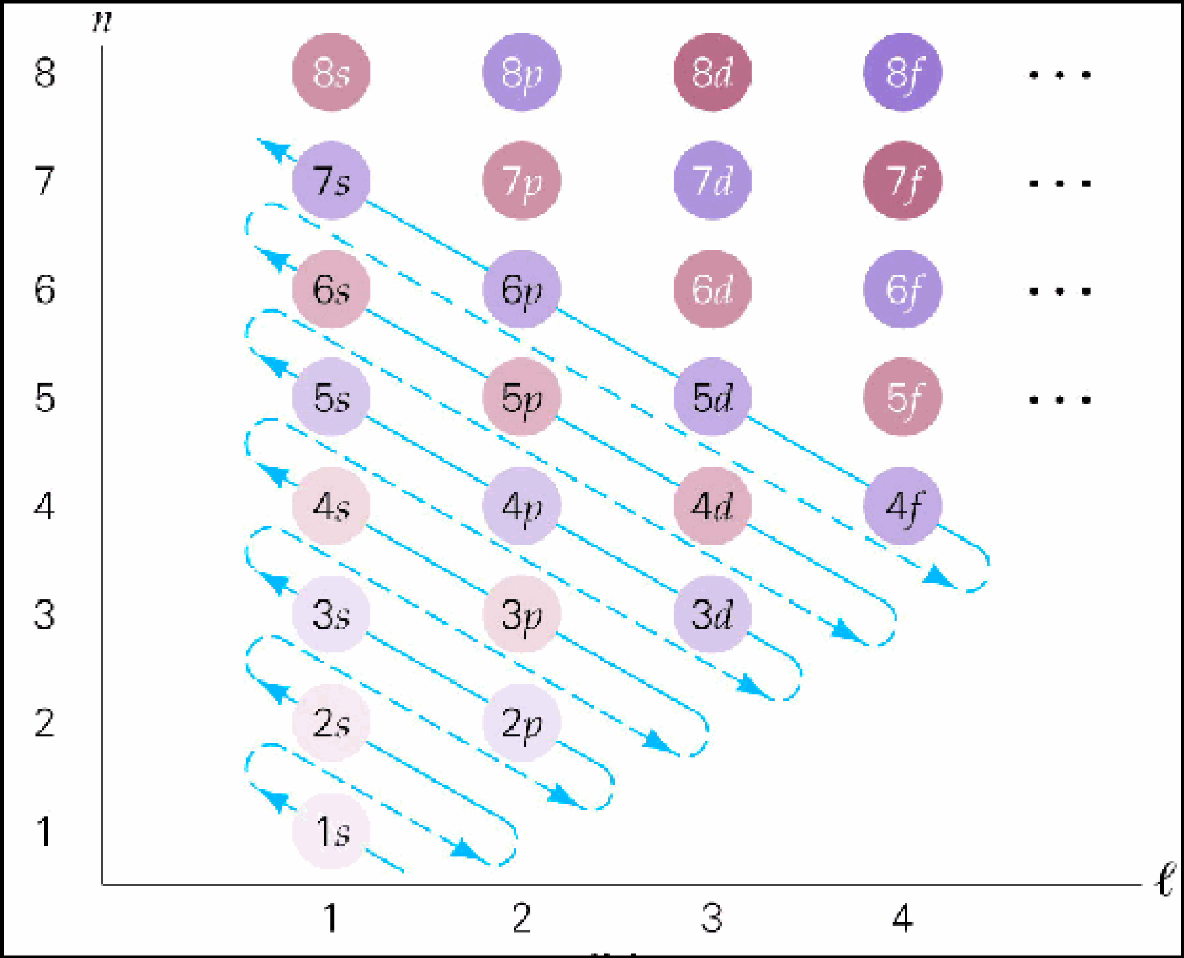
Principal Quantum Number, n = 2

n	ℓ	m_ℓ	m_s
2	0	0	+ 1/2
2	0	0	– 1/2
2	1	– 1	+ 1/2
2	1	– 1	– 1/2
2	1	0	+ 1/2
2	1	0	– 1/2
2	1	1	+ 1/2
2	1	1	– 1/2

element	Z	configuration
H	1	$1s$
He	2	$1s^2$
Li	3	$1s^22s$

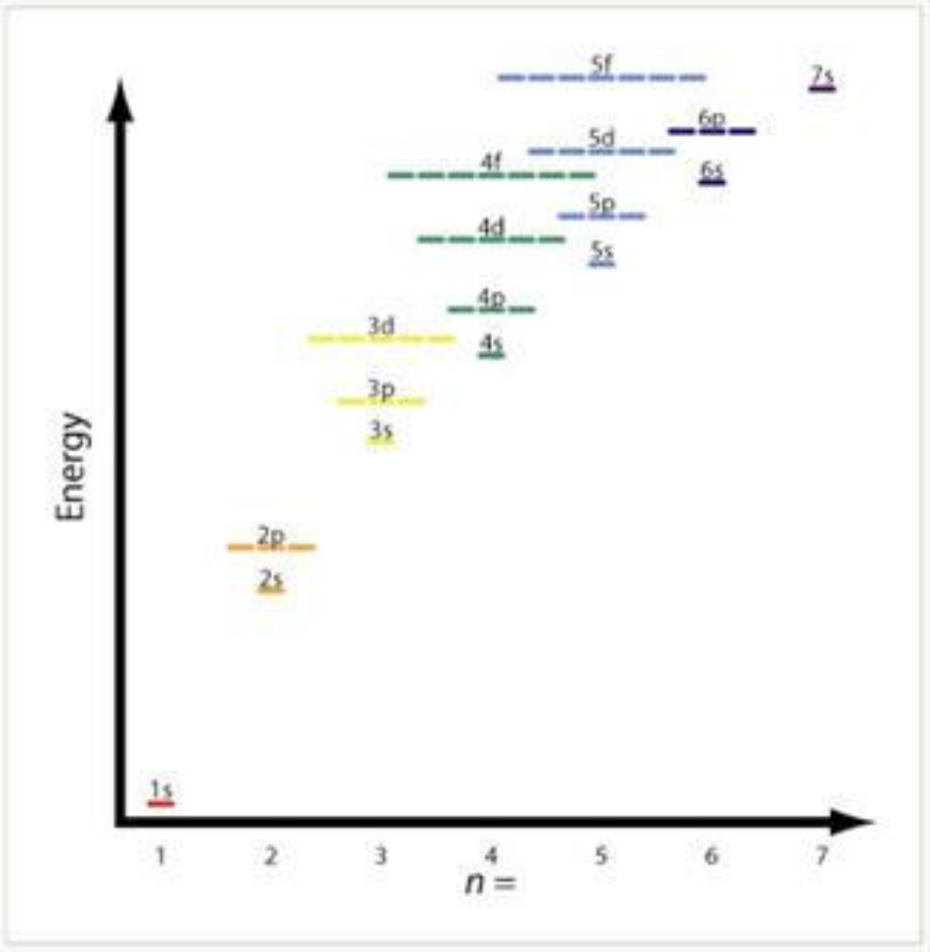
Li	3	$1s^22s$
Be	4	$1s^22s^2$
B	5	$1s^22s^22p$
C	6	$1s^22s^22p^2$
N	7	$1s^22s^22p^3$

„Aufbau“ Principle (I)



„Aufbau“ Principle (II)

Lecture 1 – **Atoms** – QM Model



„Aufbau“ Principle (III)

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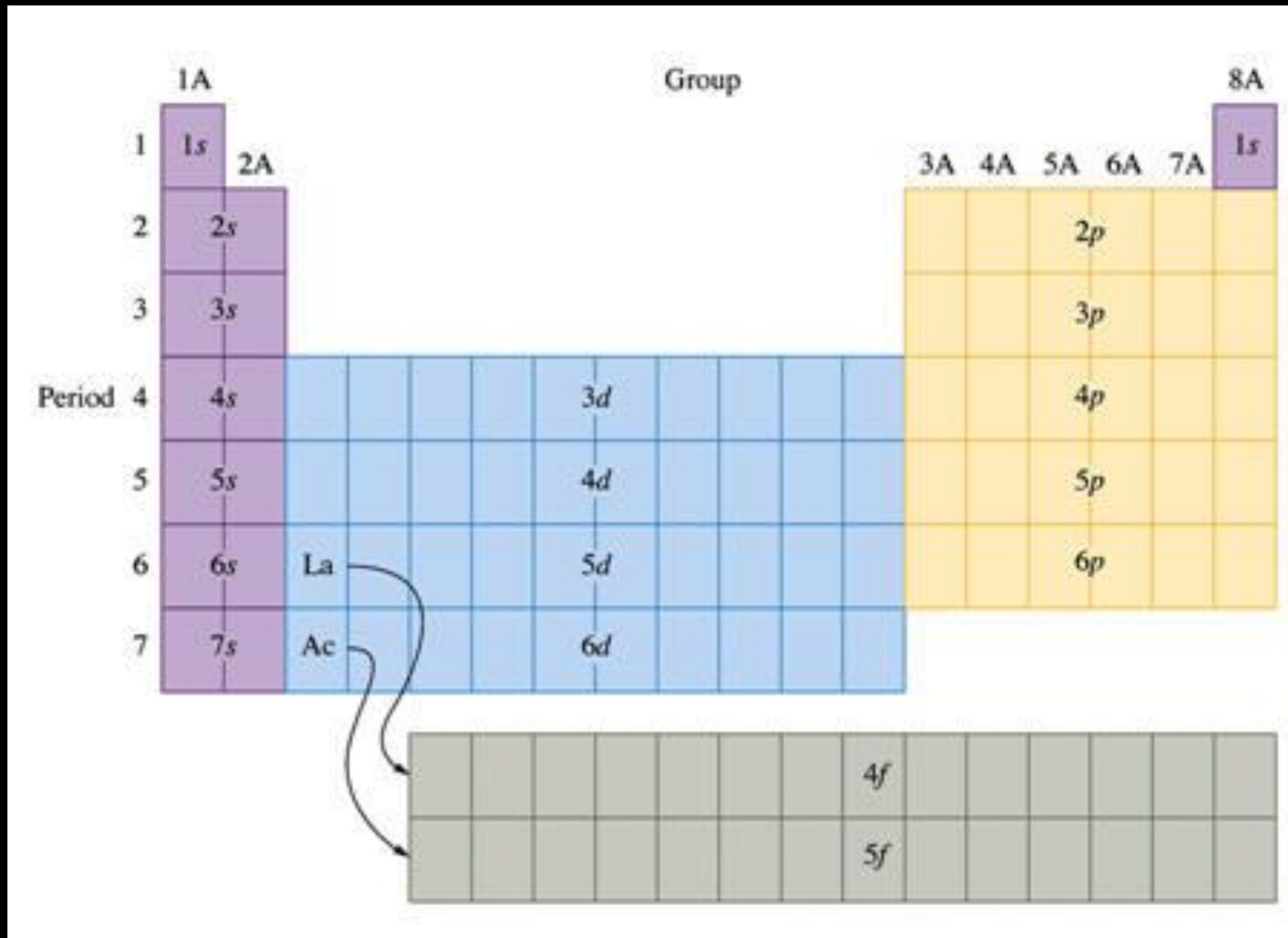
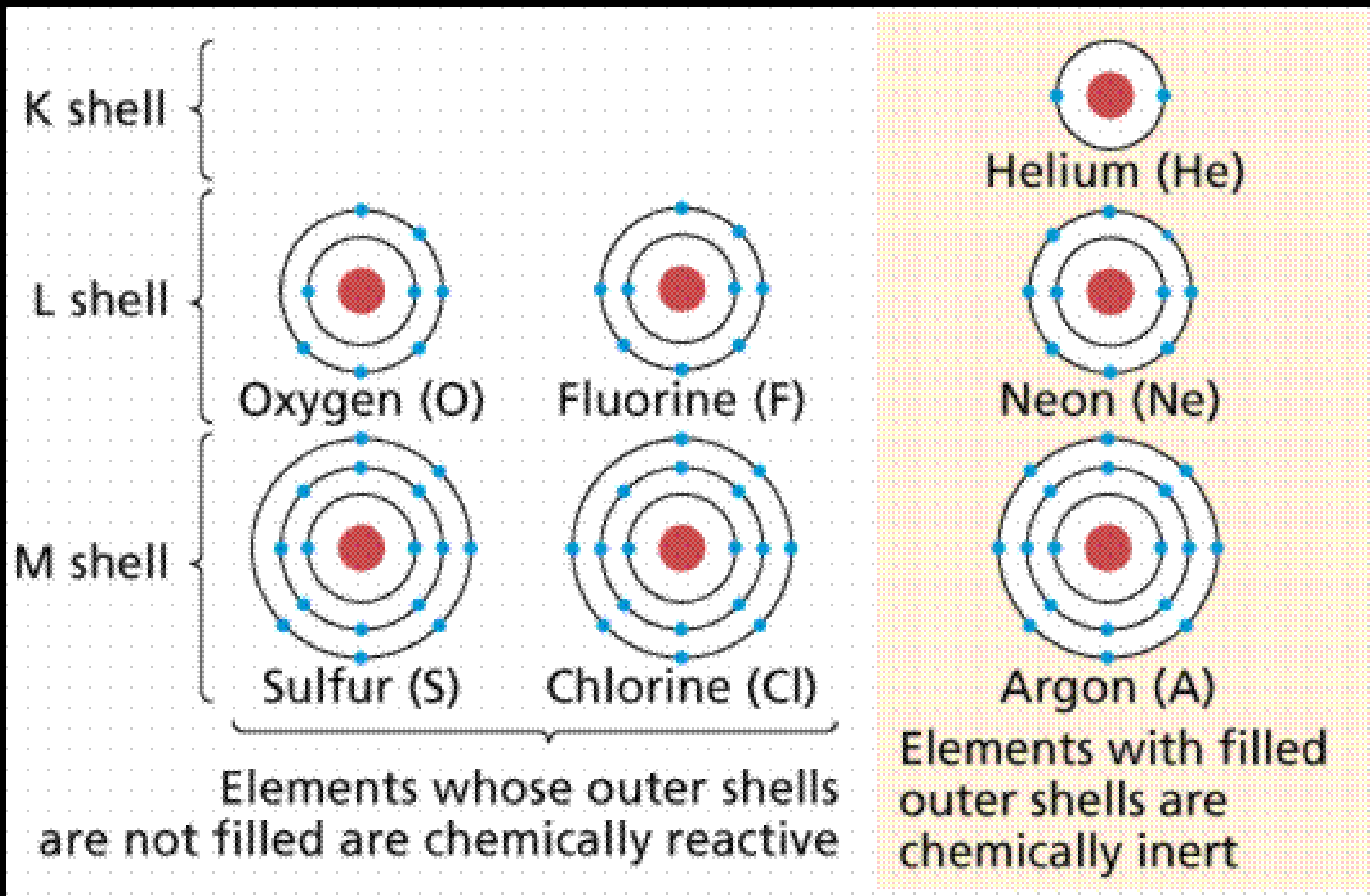
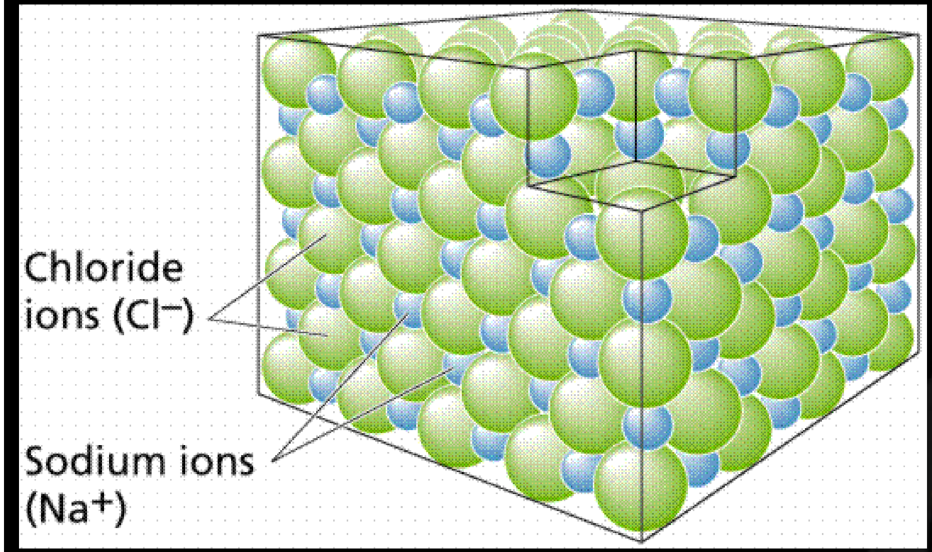


„Aufbau“ Principle (IV)



Chemical Properties

Lecture 1 – Atoms – QM Model



Molecules, Crystals, …

Lecture 1 – **Atoms** – Summary

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Atoms are the building blocks of matter; they are not fundamental but comprised of **electrons** (atomic shell) and a **nucleus** (with protons and neutrons);

Much about the **structure of atoms** has been learned from the **light** (emitted or absorbed by them), and from the structure, deep insight has been obtained about the basic underlying physics;

The **number of protons** in the nucleus fixes the **chemical element**. The **atomic shell** (structure) largely determines the characteristics of the elements, e.g., their **chemical properties**;

With the help of the **Pauli (Exclusion) Principle**, the Table of Elements can be constructed.

→ **Why does the Table of Elements end ?** → Next lecture!

გმადლობთ