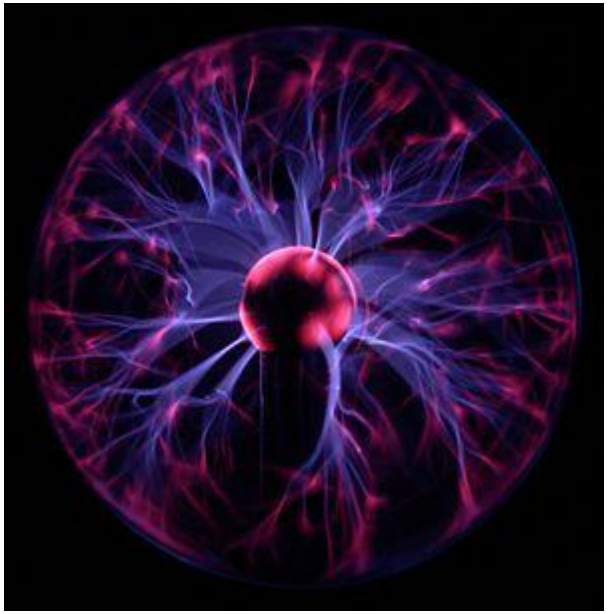
Basic Atomic Theory



EE 403/503

Introduction to Plasma Processing

September 7, 2011

Outline

1- Summary

2- Introduction to Atomic Theory

- Bohr’s Atomic Model
- Quantum Mechanical Model

3- Some Definition

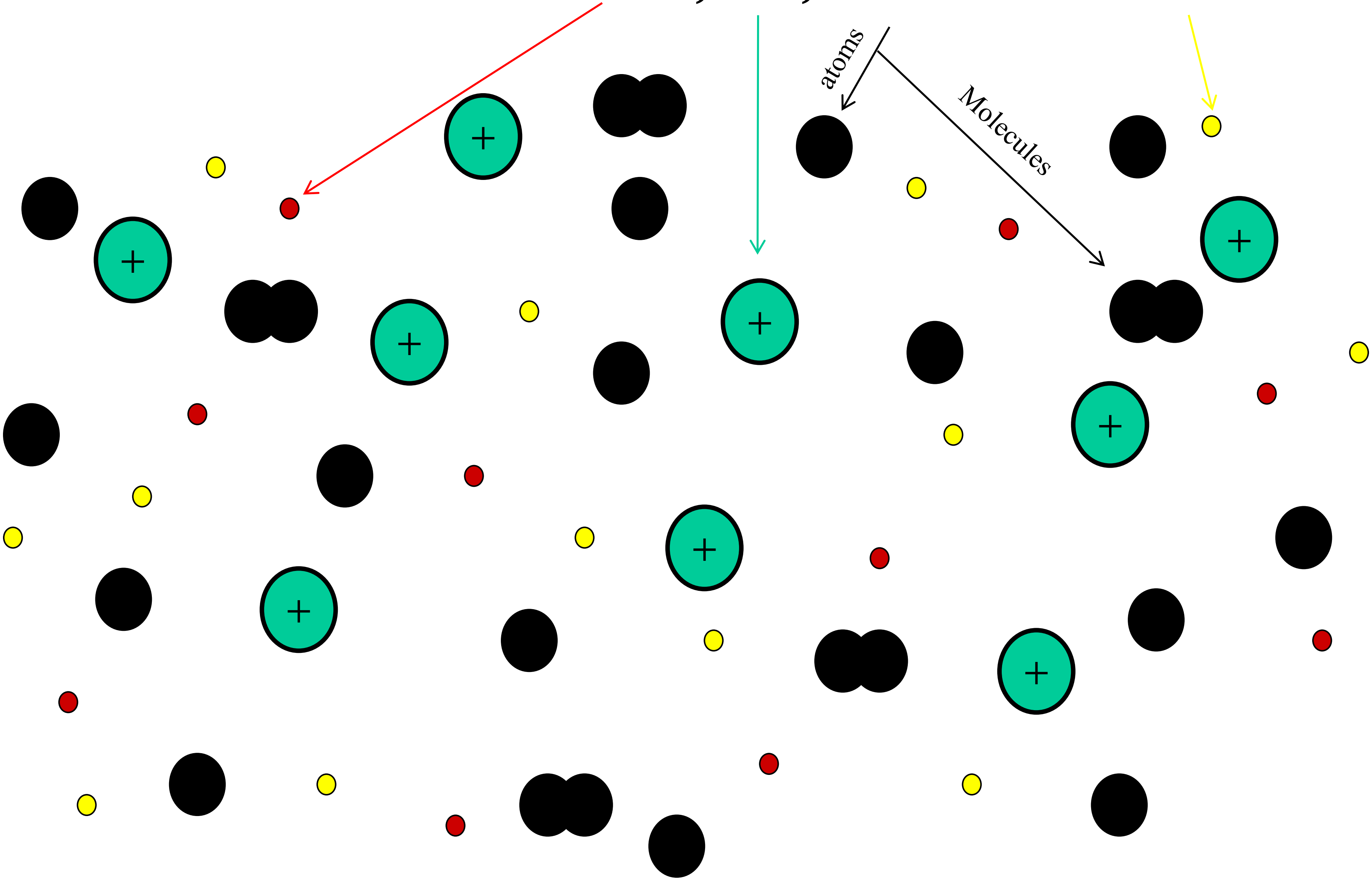
- Temperature
- Pressure

3- Projects

- Website
- Subject Areas

Summary

Plasma is a Mixture of electrons, ions, neutrals and Photons



Plasma Species

(Structures and Properties)

Electrons:

mass=9.11 x 10^{-31} Kg, Charge=1.602 x 10^{-19} C and

$F=e(E+v \times B)$ Lorentz Force

Photons:

$E=h\nu$, $c=\lambda\nu$ and $p=h/\lambda$

$h=6.626 \times 10^{-34}$ Js $c=3\times10^{8}$ m/s

Neutrals:

Atoms & molecules have internal structure

Therefore, they have **kinetic** + **internal** energies

Ions: Almost the same mass as neutrals

Positive (H^+ & Cl_2^+) and negative ions (O_2^- & SF_6^-)

Omega Centauri from Hubble Telescope

Plasma Generation

Power Supply:

Power (currents & Voltages)
Impedance
Frequency

Beams:

Laser
Electrons
ions

Materials:

Solid
Liquid
Gas

Plasma Container:

Geometry
Pressure
contaminations

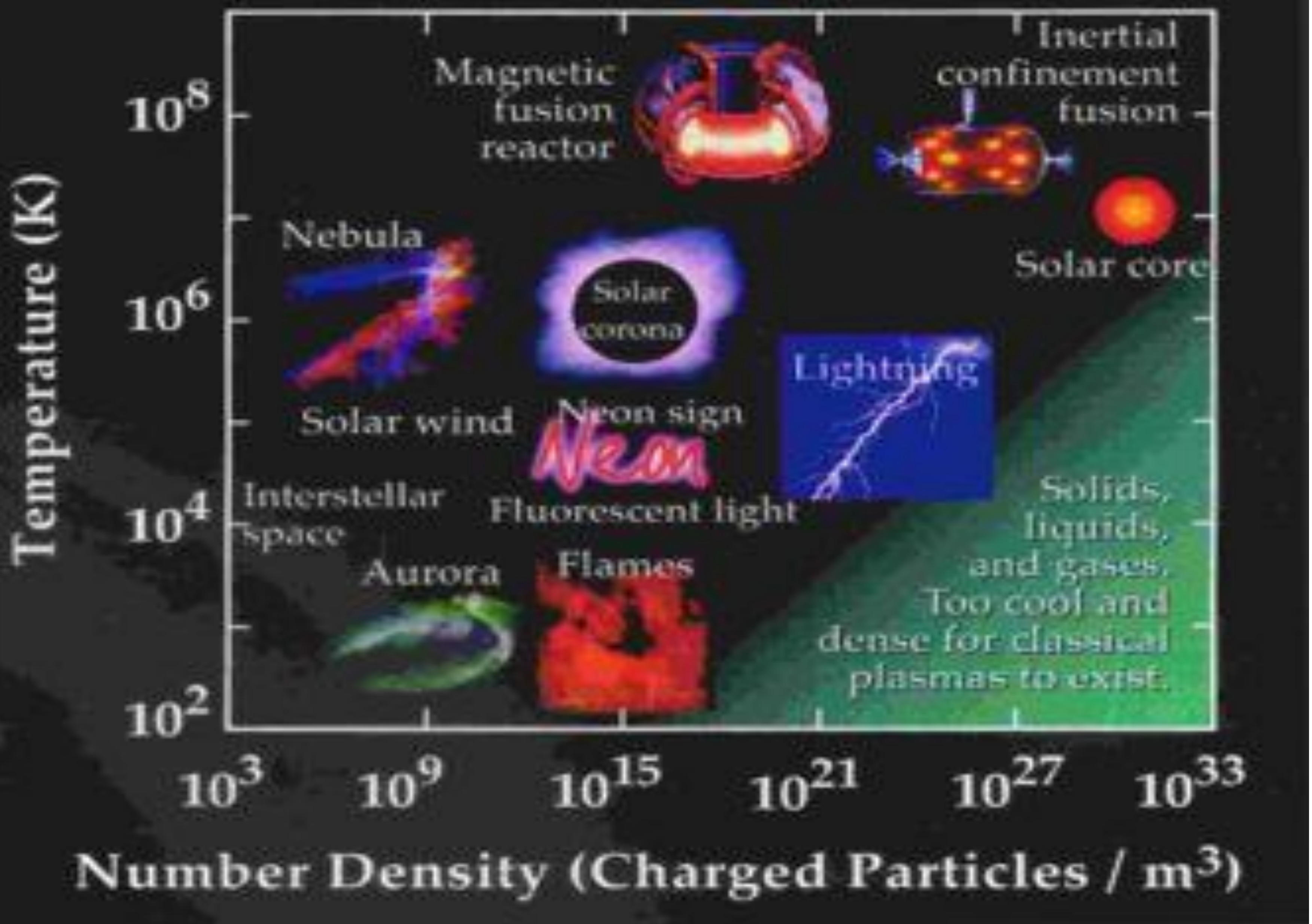
Plasmas:

Concentrations
Velocity distributions
(or temperatures?)

Properties

Thermodynamic:
enthalpy, entropy, internal energy, free energy, …
Transport:
viscosity, electrical and thermal conductivity, mobility, …

Plasmas - The 4th State of Matter

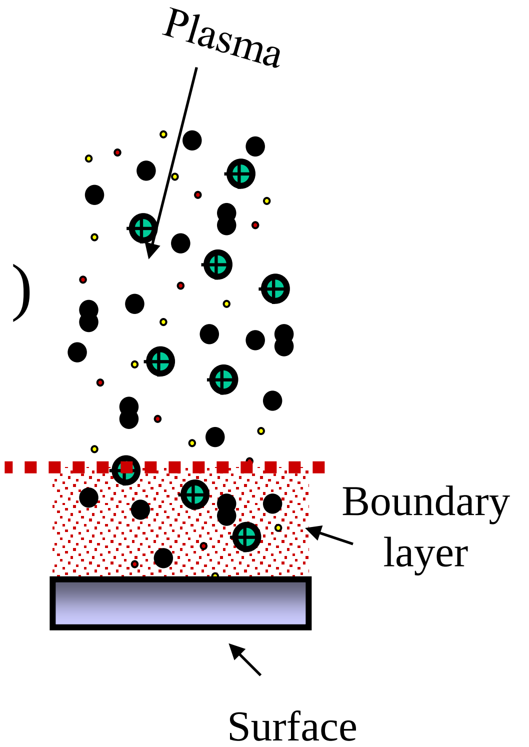


Understanding of plasma and plasma-surface interaction is essential in working with and improving plasma processing applications.

Plasma

- Species concentrations
- Velocity distributions of species (or temperatures?)

Species structure and properties
Interactions among species
Species response to external fields (electric and magnetic)



Plasma-Surface Interactions

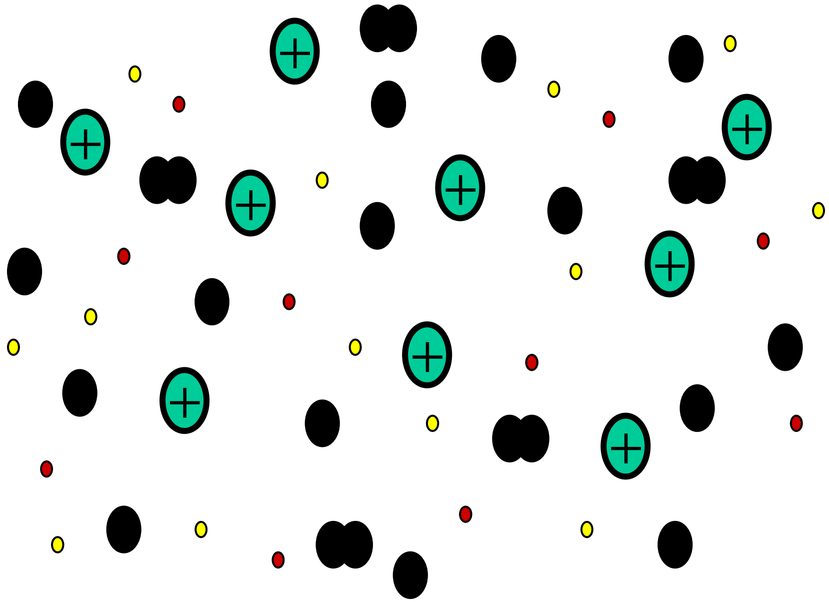
Variations of species concentrations and velocity distributions in the boundary layer between plasma and surfaces

The order of our studies:

1- Species structure and properties
2- Interactions among species
3- Species reactions to external fields (electric and magnetic)
4- Species temperatures (or velocity distributions)
5- Species concentrations
6- Plasma-Surface Interaction
7- Plasma Characteristics
8- Plasma Discharges
9- Plasma Applications

What is Temperature in an ideal gas?

$$E = \frac{3}{2}kT = \frac{1}{2}m\overline{v^2}$$



$$T = f(v)$$

E1-Example 1:

<u>How fast is an Electron and a Hydrogen atom at room temperature?</u>

$$\frac{3}{2}kT = \frac{1}{2}m\overline{v^2}$$

$$v = \sqrt{\frac{3kT}{m}}$$

$$v = 1.2\times10^5\, m/s$$

<u>Hydrogen:</u>

m_H = 1.66 x 10^{-27} Kg
k = 1.38 x 10^{-23} J/K (Boltzmann's Constant)
T = 293K

$$v_{rms} = \sqrt{\frac{3kT}{m}}$$

$$v_{rms} = 2703 \quad m/s$$

Problem 1

A helium non-thermal plasma used in biomedical applications, the gas temperatures are close to room temperatures. However, the electrons have average energies around 3 eV. Find the average velocity of electrons, He and He^+.

m_{He}=6.65x10^{-27}Kg ; $\bar{v} = 0.9213 \times v_{rms}$

$$E = \frac{3}{2}kT = \frac{1}{2}m\overline{v^2}$$

$$v_{rms,He} = \sqrt{\frac{2E_{He}}{m_{He}}} = \sqrt{\frac{3kT_{He}}{m_{He}}} = \sqrt{\frac{3\times1.38\times10^{-23}\times293}{6.65\times10^{-27}}}$$

$$v_{rms,He} = 1.35\times10^{3} \quad m/s \quad \Rightarrow \quad \boxed{\bar{v}_{He} = 0.9213\times v_{rms,He} = 1.24\times10^{3}}$$

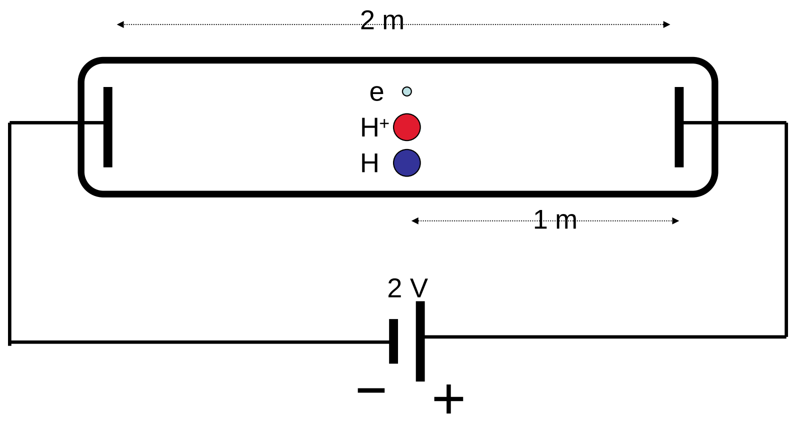
$$v_{rms,He^{+}} = v_{rms,He} \quad m/s$$

$$v_{rms,e} = \sqrt{\frac{2E_e}{m_e}} = \sqrt{\frac{2\times3\times1.6021\times10^{-19}}{9.1\times10^{-31}}} = 1.03\times10^{6} \quad m/s$$

$$\boxed{\bar{v}_e = 9.47\times10^{5} \quad m/s}$$

E1: Example 2

In the vacuum tube shown in the figure below, determine the location, velocity and energy of e, H and H+ at the time when the electron arrives at one of the electrodes. All three particles are initially at rest.



$$F = ma$$

$$\Downarrow$$

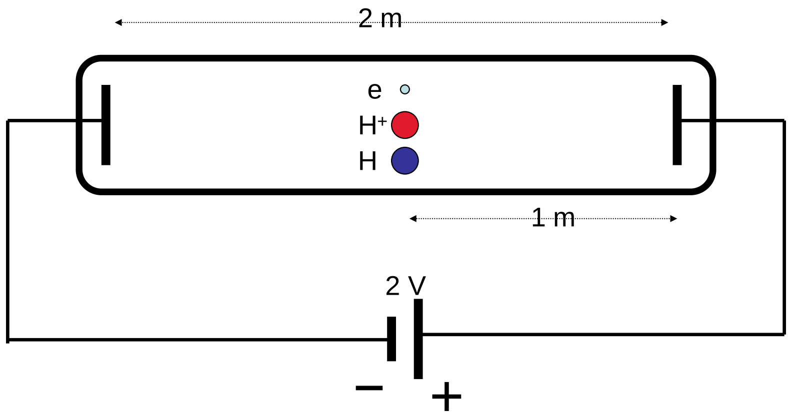
$$a = \frac{F}{m}$$

$$F = qE$$

$$V = E \times d \quad \Rightarrow \quad E = \frac{V}{d}$$

$$x = \frac{1}{2}at^2 = \frac{1}{2}\left(\frac{F}{m}\right)t^2 = \frac{1}{2}\frac{qE}{m}t^2 = \frac{1}{2}\frac{q\left(\frac{V}{d}\right)}{m}t^2 = \frac{qV}{2md}t^2$$

Determine the location, velocity and energy of e, H and H+ at the time when the electron arrives at one of the electrodes. All three particles are initially at rest.



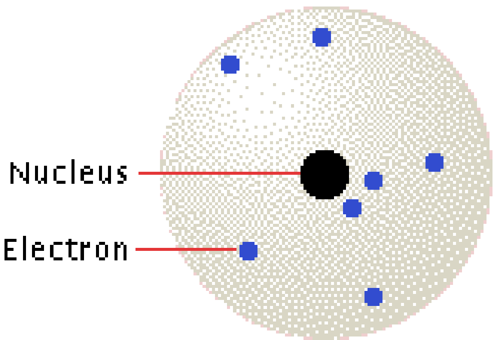
$$x = \frac{1}{2}at^2 = \frac{qV}{2md}t^2$$

$$x_e = \frac{1.6\times10^{-19}\times2}{2\times9.11\times10^{-31}\times2}t_e^2 = 1 \quad \Rightarrow \quad t_e = 3.4\times10^{-6}$$

$$x_{H^+} = \frac{1.6\times10^{-19}\times2}{2\times1.66\times10^{-27}\times2}\times\left(3.4\times10^{-6}\right)^2 = 5.57\times10^{-4}$$

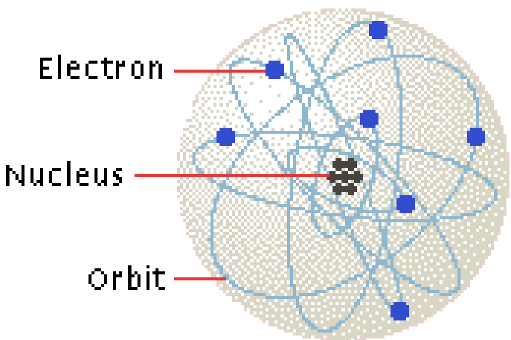
$$x_H = 0$$

Structure of an Atom



The Rutherford Model pictured the atom as a miniature solar system with the electrons moving like planets around the nucleus. (1871-1937)

The s orbital: Electrons with no angular momentum occupy regions of space like this. Shading shows probability of finding an electron at that distance.



The Bohr Model (1885-1962) 'quantized' the orbits in order to explain the stability of the atom.

The Schrödinger Model abandoned the idea of precise orbits, replacing them with a description of the regions of space (called orbitals) where the electrons were most likely to be found. (1887-1961)

The Structure of Atoms

(6:11 Min)

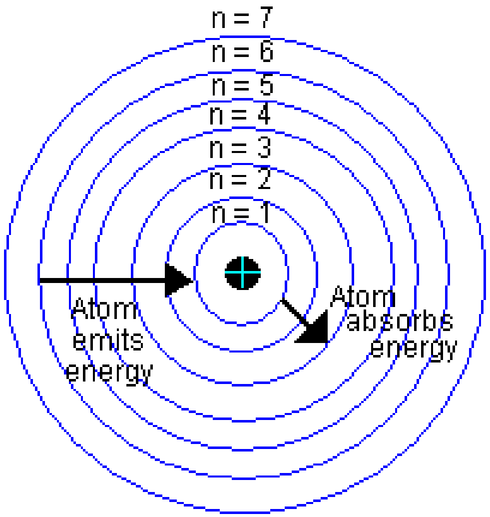
Quantum Mechanics: The Uncertainty Principle

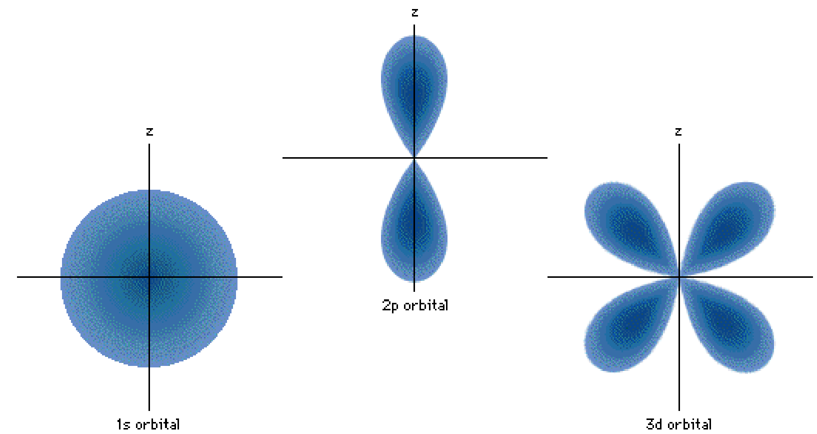
(5.48 Min)

Bohr's Theory

Quantum Mechanics

(Schroedinger Equation)





$$\Delta E = R_H\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

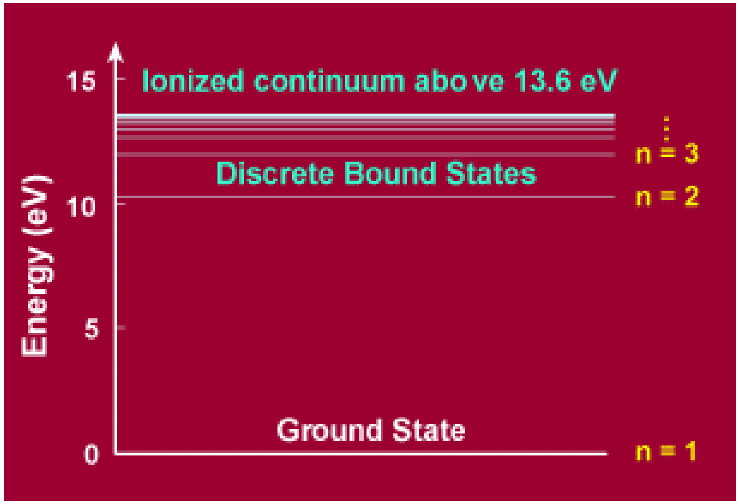
Rydberg constant

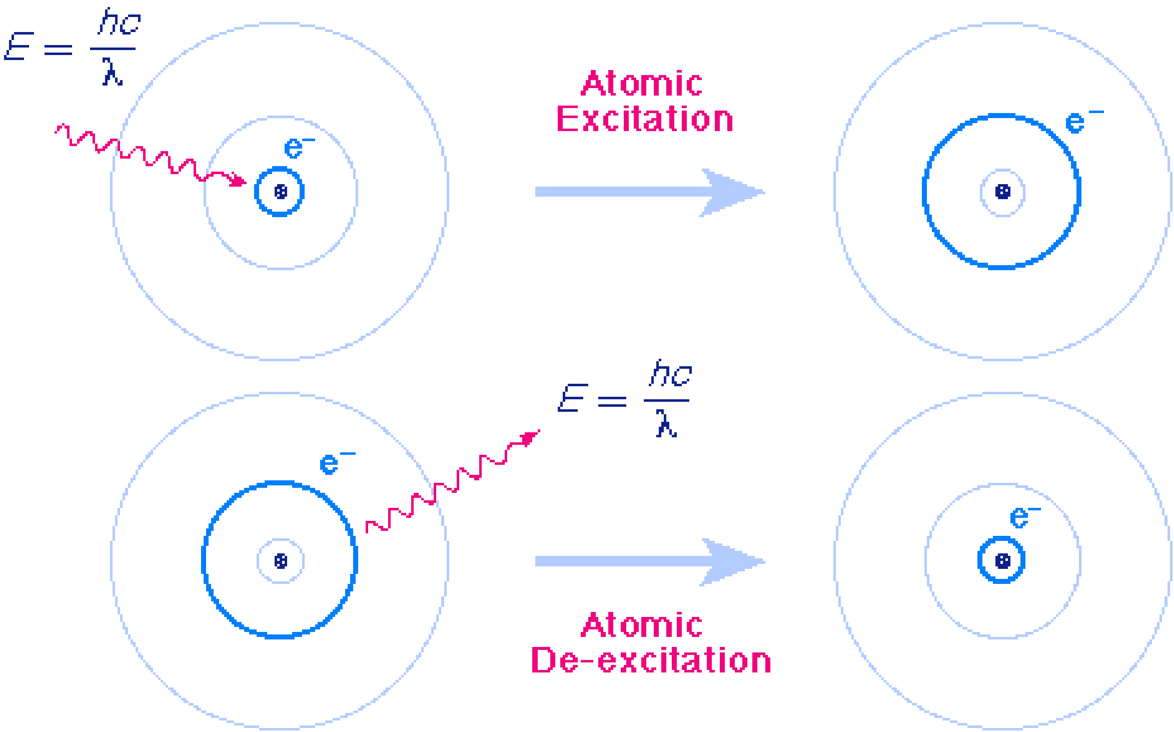
$$i\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V(\mathbf{r})\psi(\mathbf{r},t)$$

$$E_n = 13.5992\left(1 - \frac{1}{n^2}\right) \quad [eV]$$

$$< A >= \int \psi^*(\mathbf{r},t)\hat{A}\psi(\mathbf{r},t) = \int \psi^*(\mathbf{r})\hat{A}\psi(\mathbf{r})$$

Bohr's Theory

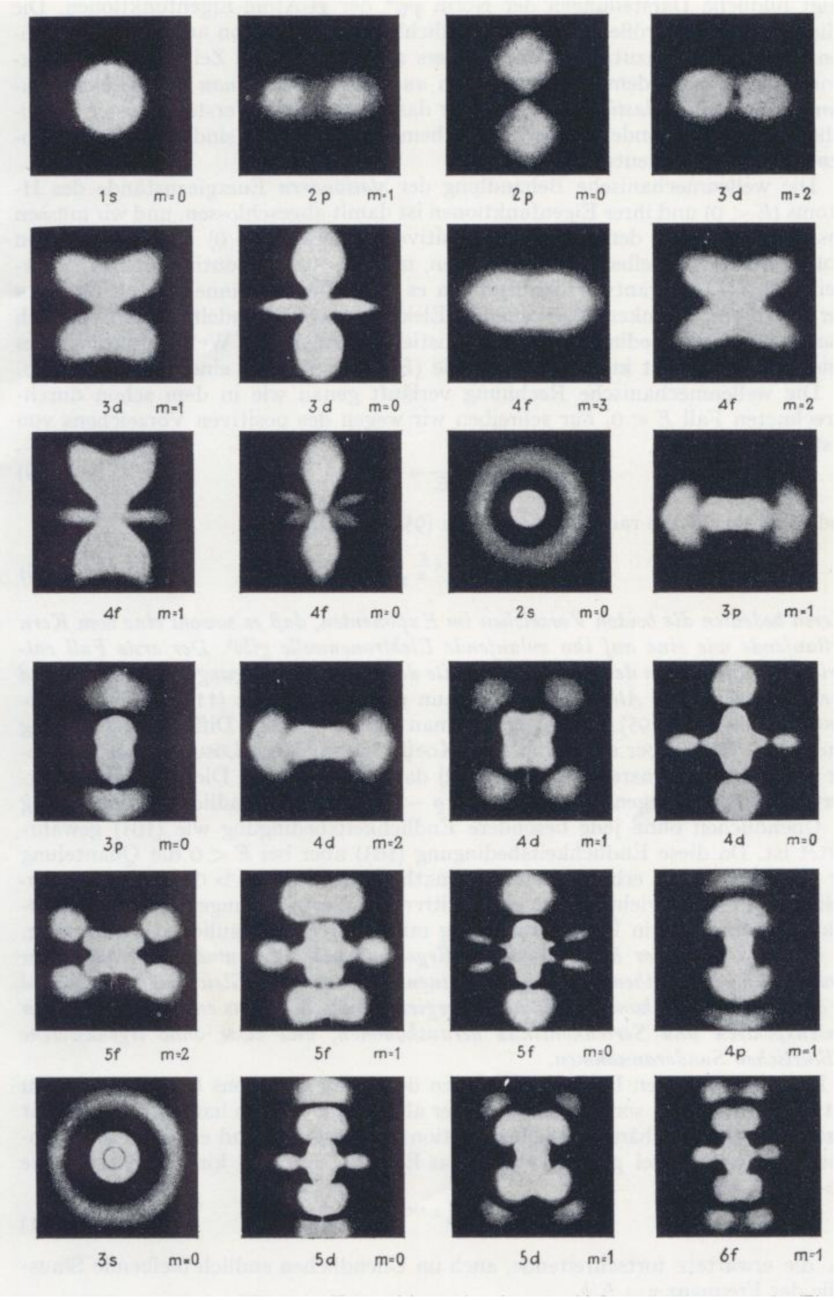




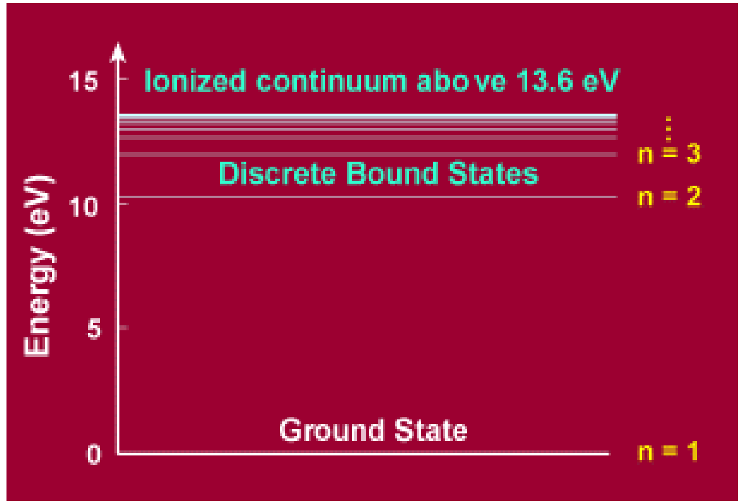
Quantum Mechanics

Schrödinger & Bohr Atomic Models

Structure of Hydrogen Atoms



E1-Example 3



Calculate the five lowest energy states including the ground state of hydrogen atoms in eV.

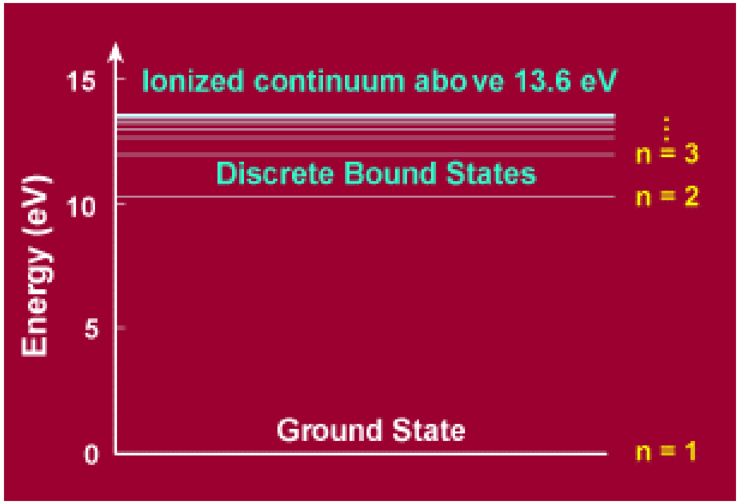
Calculate the ionization potential of hydrogen atoms in eV.

Find the energy states of hydrogen atoms that can absorb photons with wavelengths in the visible range (400-700 nm).

Calculate the five lowest energy states including the ground state of hydrogen atoms in eV.

$$\Delta E = R_H \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

$$E_n = 13.5992 \left(1 - \frac{1}{n^2} \right) \quad [eV]$$



$$n = 1 \qquad E_1 = 0 \qquad [eV]$$

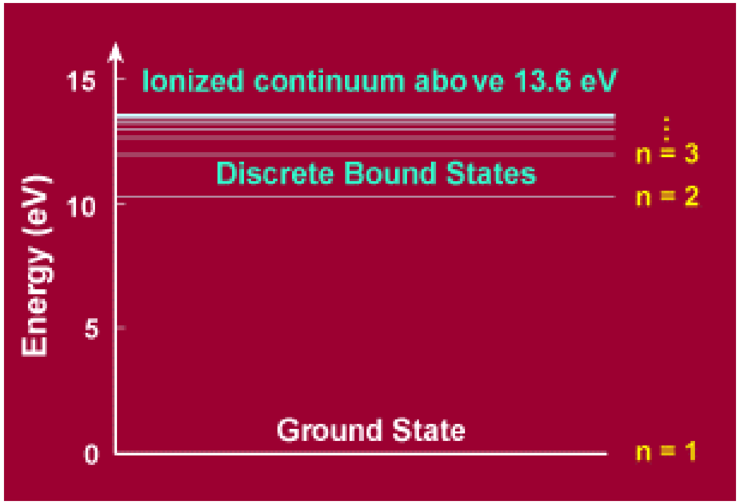
$$n = 2 \qquad E_2 = 10.2$$

$$n = 3 \qquad E_3 = 12.1$$

$$n = 4 \qquad E_4 = 12.7$$

$$n = 5 \qquad E_5 = 13.1$$

Calculate the ionization potential of hydrogen atoms in eV.



$$E_n = 13.5992\left(1 - \frac{1}{n^2}\right) \quad [eV]$$

$$n = \infty \qquad E_{ionization} = 13.5992 \quad [eV]$$

Find the energy states of hydrogen atoms that can absorb photons with wavelengths in the visible range (400-700 nm).

$$E = h\nu = \frac{hc}{\lambda} = \frac{6.626\times10^{-34}\times3\times10^{8}}{\lambda\times10^{-9} \quad [nm]} = \frac{1.9878\times10^{-16}}{\lambda} \quad [J] = \frac{1240}{\lambda} \quad [eV]$$

$$\lambda = 400nm \quad \Rightarrow \quad 3 \quad [eV]$$

$$\lambda = 700nm \quad \Rightarrow \quad 1.8 \quad [eV]$$

$$n=1 \qquad E_1 = 0 \quad [eV]$$

$$n=2 \qquad E_2 = 10.2$$

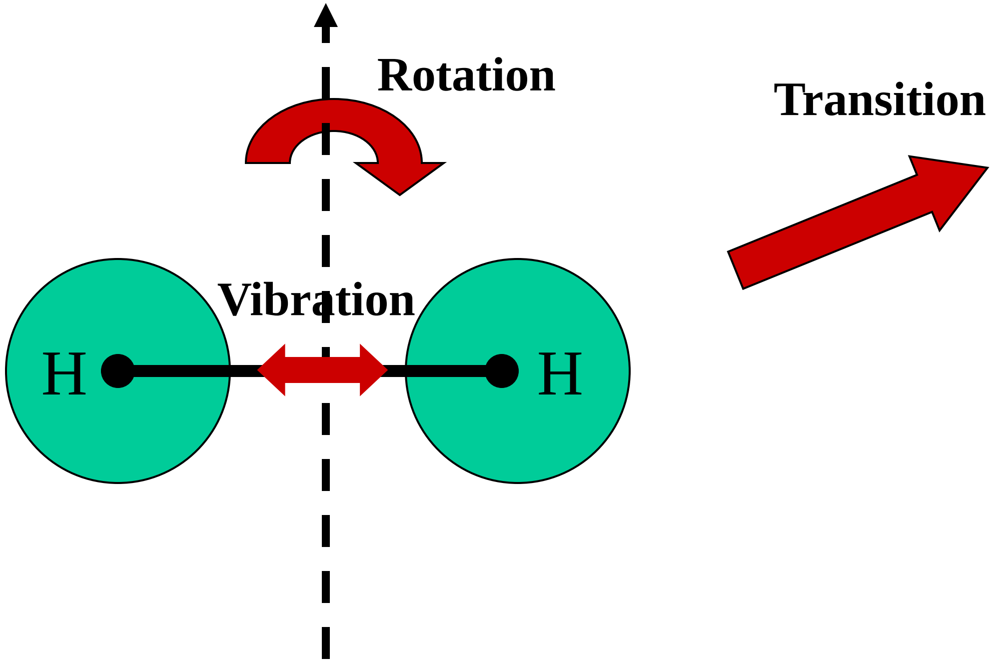
$$n=3 \qquad E_3 = 12.1$$

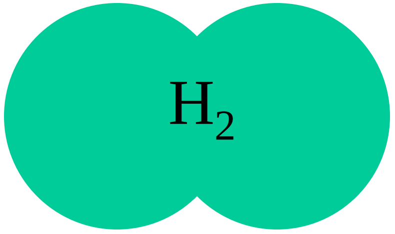
$$n=4 \qquad E_4 = 12.7$$

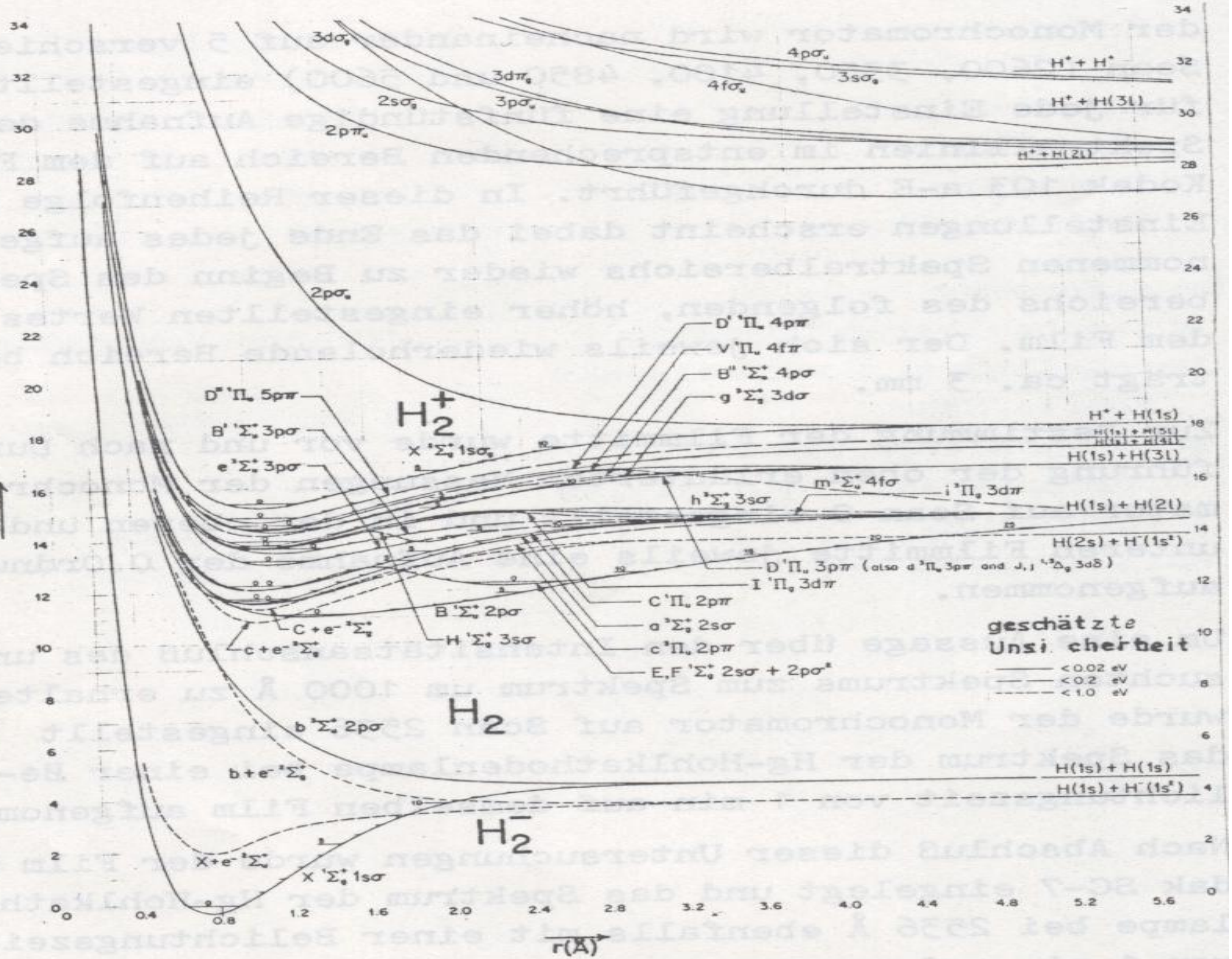
$$n=5 \qquad E_5 = 13.1$$

$$n_{upper} = 3,4,5,\ldots \quad \rightarrow \quad n = 2$$

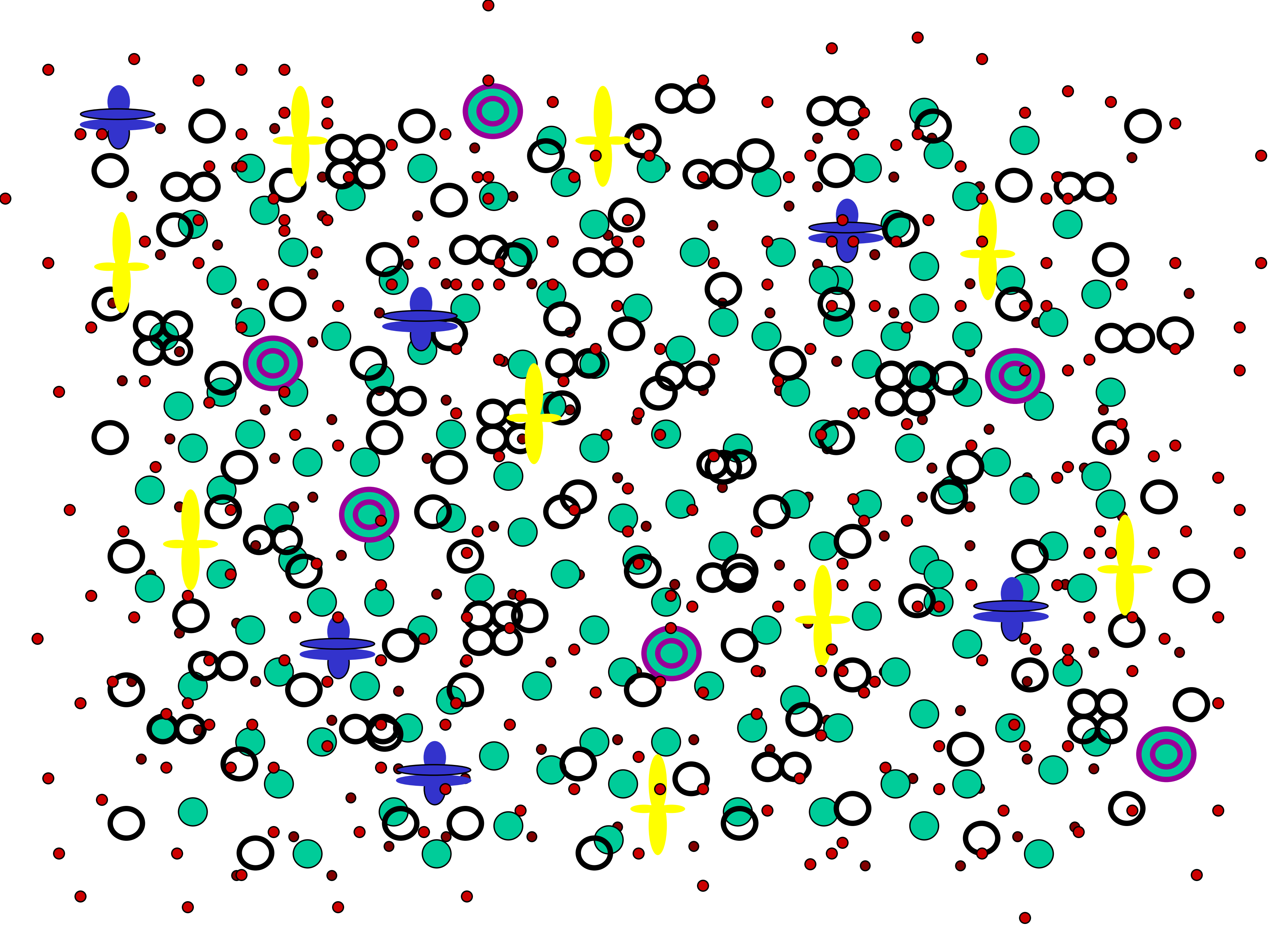
Hydrogen Molecule







3dσg
4pσu
H⁺ + H⁺
3dπg
3sσg
4fσu
2sσg
3pσu
H⁺ + H(3l)
2pπu
H⁺ + H(2l)
2pσu
H2+
D' ¹Πu 4pπ
V ¹Πu 4fπ
B'' ¹Σu+ 4pσ
g ³Σg+ 3dσ
D'' ¹Πu 5pπ
B' ¹Σu+ 3pσ
e ³Σu+ 3pσ
X ²Σg+ 1sσg
H⁺ + H(1s)
H(1s) + H(3l)
m ³Σu+ 4fσ
i ³Πg 3dπ
h ³Σg+ 3sσ
H(1s) + H(2l)
H(2s) + H⁻(1s²)
D ¹Πu 3pπ (also d ³Πu 3pπ and J, j ¹,³Δg 3dδ)
I ¹Πg 3dπ
C ¹Πu 2pπ
B ¹Σu+ 2pσ
a ³Σg+ 2sσ
C + e⁻ ²Σu+
c + e⁻ ²Σg+
H ¹Σg+ 3sσ
c ³Πu 2pπ
E,F ¹Σg+ 2sσ + 2pσ²
geschätzte Unsicherheit
< 0.02 eV
< 0.2 eV
< 1.0 eV
H2
b ³Σu+ 2pσ
b + e⁻ ²Σg
H(1s) + H(1s)
H(1s) + H⁻(1s²)
H2−
X + e⁻ ²Σu
X ¹Σg+ 1sσ
eV
r(Å)



What is pressure of an ideal gas?

Number of particles per m^{-3}

$k=1.38\times10^{-23}$ J/K   Boltzmann Constant

Pressure

Temperature

$$p = n \times k \times T$$

[Pascal=N/m^2; 1 atm=760 Torr =101325 Pa]

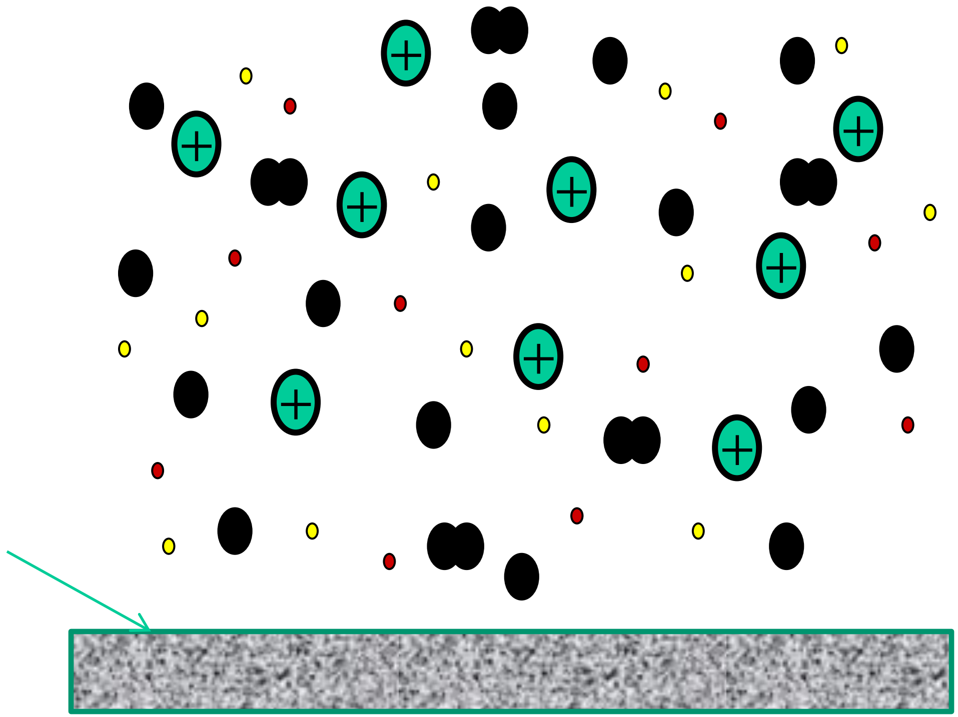
$$p = \underbrace{n_e k T_e}_{\text{Electron Partial Pressure}} + \underbrace{n_{ion} k T_{ion}}_{\text{ions Partial Pressure}} + \underbrace{n_a k T_a}_{\text{Neutral species Partial Pressure}}$$

Electron
Partial Pressure

ions
Partial Pressure

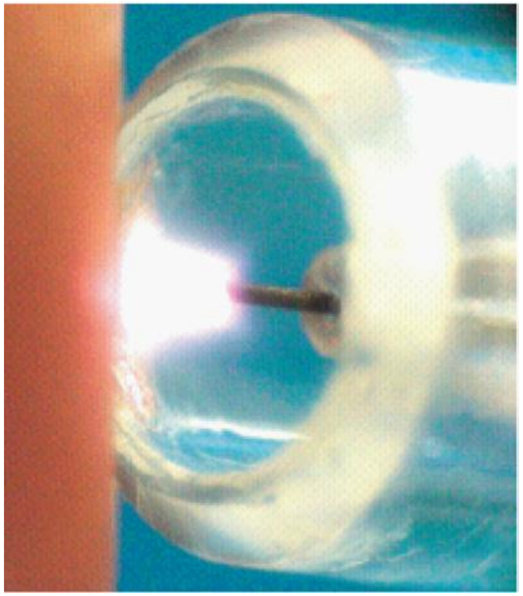
Neutral species
Partial Pressure

Total number of collision on the substrate per unit area per unit time



$$= \frac{1}{4} n\bar{v} = \frac{1}{4} n_e \bar{v}_e + \frac{1}{4} n_{ion} \bar{v}_{ion} + \frac{1}{4} n_a \bar{v}_a$$

Problem 2



How many electrons, He and He^{+} are impacted on the surface per unit area and per second. Number density of He and electrons are approximately 10^{17} and 10^{13} [m^{-3}], respectively.

Number of collisions on the substrate Per unit area and per unit time, n_c. $= \frac{1}{4} n\bar{v}$

$$n_{c,He} = \frac{1}{4} \times 10^{17} \times 1.24 \times 10^{3} = 3.1 \times 10^{20}$$

$$n_{c,He^+} = \frac{1}{4} \times 10^{13} \times 1.24 \times 10^{3} = 3.1 \times 10^{16}$$

$$n_{c,e} = \frac{1}{4} \times 10^{13} \times 9.47 \times 10^{5} = 2.4 \times 10^{19}$$

Projects