1 – Exercise on aluminum structure.

Al ($1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^1$) crystallizes in the *face-centered cubic* (*fcc*) Bravais lattice with a lattice parameter a = 4.05 Å. Al mass density is 2.7 g/cm^3 and atomic mass is 27 g.

a. Calculate the atomic concentration per cm^3 using two different ways.
b. Calculate the electronic concentration per cm^3.
c. Deduce the radius of the Fermi sphere and give the value of the Fermi energy in eV. Express the Fermi energy in Kelvin.
d. Draw the primitive translation vectors of the *fcc* lattice and write them as a linear combination of the edge length a of the convention cell. Write the volume of the primitive cell in terms of a.
e. Write the primitive translation vectors of the reciprocal lattice to the *fcc* lattice. Check that these are primitive translation vectors of a *body-centered cubic* (*bcc*) lattice. Draw the first Brillouin zone of the *fcc* lattice.
f. We consider the Bragg plane limiting the 1st Brillouin zone in the k_x direction. Write the free-electron energy for the states belonging to this Bragg plane versus k_y and k_z. Give a graphic representation of $E(k_y,k_z)$ and determine its minimum value (in eV).

2 - Exercise on graphene structure.

a. Determine the Bravais lattice of the honeycomb structure of graphene (crystalline structure of C atoms in graphene). Calculate the area of the Bravais lattice as a function of $a_{C\text{-}C}$ = distance between two C neighboring atoms ≈ 1.42 Å.
b. Write the single electron functions entering sp_i^2 hybridized orbitals of graphene as linear combinations of the base orbitals $\left|sp_i^2\right\rangle = \alpha_i\left|2s\right\rangle + \beta_i\left|2p_x\right\rangle + \gamma_i\left|2p_y\right\rangle$ with i = 1, 2 or 3. These orbitals should satisfy orthonormalization conditions. Derive the angle in the graphene plane formed between σ bonds involving sp^2 orbitals of 3 adjacent atoms.

3 – Exercise on collision time

Consider a molecule with velocity v. Let

$P(t)$ = the probability that such a molecule survives a time t without suffering a collision. To describe the collisions, let

$w\,dt$ = the probability that a molecule suffers a collision between time t and $t + dt$, dt being an infinitesimal time later. The quantity w is the probability per unit time that a molecule suffers a collision, and is called the collision rate. We shall assume that the probability w is *independent* of the past history of the molecule and for simplicity we shall assume that w does not depend on the speed v of the molecule under consideration.

a. Calculate the probability $P(t)$ of surviving a time t without suffering a collision. We will impose the condition $P(0) = 1$ since a molecule has no chance of colliding in a time $t \to 0$.
b. Calculate the probability that the molecule, after surviving without collisions for a time t, suffers a collision in the infinitesimal time interval between t and $t + dt$.
c. Check that the probability calculated in b. is properly normalized. This asserts simply that there is a *probability unity* that the molecule collides at *some* time.
d. Let τ be the mean time between successive collisions. This is called the collision time or relaxation time of the molecule. Using the probability found in b., show that the collision time is the inverse of the collision rate. The mean distance traveled by such a molecule between collisions is called the mean free path l of the molecule. One has thus $l = v\ \tau$. A gas of molecules can then be conveniently characterized by the average collision time, or the average mean free path of the molecules traveling with a speed v.
e. Can the collision model for a gas of molecules be transposed for a gas of electrons? What is the name of the model developed at the beginning of the twentieth century?

4 – Exercise on the kinetic theory of gases

The kinetic theory of gases relates the macroscopic properties of gases (pressure and temperature) to the microscopic properties of gas molecules (speed and kinetic energy).

We consider an **ideal gas** a gas with a low enough density – that is under conditions in which its molecules are far enough apart that they do not interact with one another. So the energy of the molecules of mass m is their kinetic energy.

a- The pressure exerted by the gas on a vessel wall of surface S is due to the molecular collisions with the wall. Assuming that any collision of the molecules with the wall is elastic (the wall is considered as a perfect mirror), determine for each molecule its change of momentum along the axis perpendicular to the surface.

b- Taking into account the concentration of molecules per unit volume, determine the number of collisions per unit time on the surface *S*.

c- Remembering that the gas is isotrope and that all molecules have not the same speed ***v***, calculate the total force exerted by the gas on the wall of surface *S*, then the pressure.

d- We have established a relation between the pressure, the volume and the total translational kinetic energy. This relation is called the *Bernoulli formula*.

e- The *absolute temperature T* is defined from a microscopic point of view versus the translational kinetic energy of a molecule, by the relation $1/2m\langle v^2\rangle = 3/2\, kT$ where k is the Boltzmann constant. Using the *Bernoulli formula*, write the **ideal gas law**. This relation may be considered as a macroscopic definition of the absolute temperature.