Q1. Graphene is a 2D crystal with carbon atoms arranged in a honeycomb structure as shown below.



Using the above information and picture, answer the following questions

- a. Assuming that the unit cell is a hexagon of carbon atoms, how many atoms of carbon are there in each unit cell?
- b. What are the basis vectors needed to reproduce the whole crystal in 2D space?
- Q2. Find the number and relative positions of all nearest and second-nearest neighbours of a lattice point in a simple cubic Bravais lattice.
- Q3. Packing fraction in two dimensions: A two-dimensional crystal is constructed by packing circles. The ratio between the area occupied by the circles and the total area is referred as the packing fraction in two dimensions. Find the packing fraction for a two-dimensional square Bravais lattice.

Repeat the same calculation for a two-dimensional triangular lattice. Which one of the two is more closely packed?

Q4. Show that the angle between two planes (or two directions) is $\cos(\theta) = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \sqrt{h_2^2 + k_2^2 + l_2^2}}$

 $[h_i, k_i, l_i]$ are the miller indices of the two planes, where i = 1, 2

- Q5. For silicon (Fig. 1.5a in ASF), answer the following questions:
 - a. How many Si atoms per sq. cm are there on a (100) plane?
 - b. How many on a (110) and (111) plane?
- Q6. The density of BCC iron is 8,000 kg/m³. Determine the lattice constant of the cubic unit cell.
- Q7. Visualize a zinc blende crystal system from three different directions [100], [110], [111] taken from three different crystal cuts.
 Utilize the Crystal Viewer Tool in ABACUS on nanoHUB. The tool can be found at: <u>https://nanohub.org/tools/abacus</u> (you will need a free nanoHUB login)