Week 03

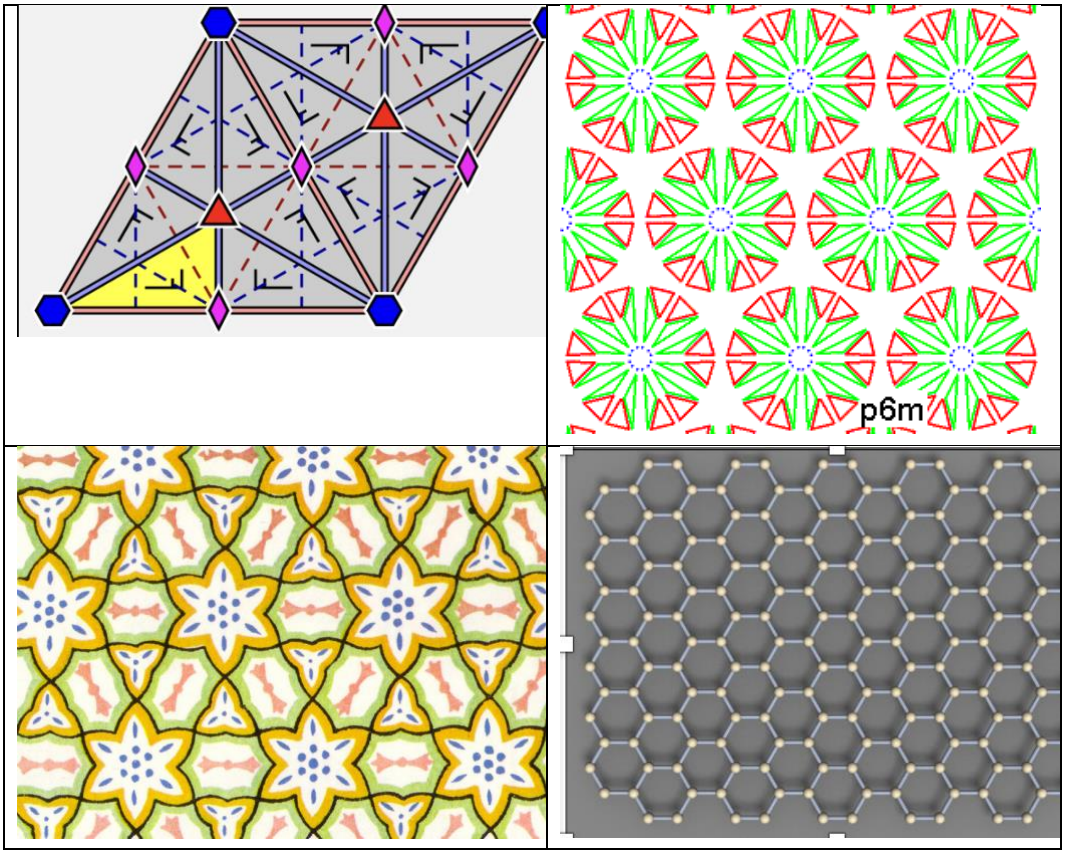
Crystallography
Symmetry

Exercise 1 : Answer these questions by true or false

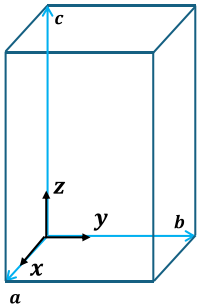
	True	False
1. In a crystal, a motif always has the same symmetry as the Bravais Lattice.	☐	☐
2. A motif with a 5-fold symmetry can be put in a Bravais lattice such that the resulting crystal has also a 5-fold symmetry.	☐	☐
3. A crystal with one atom per motif has the symmetry of its Bravais Lattice.	☐	☐
4. There are more point groups in 3D than there are point groups in 2D.	☐	☐
5. A material with only one type of atom in the motif has the same or more symmetries than a material with the same structure but atoms of different nature in the motif.	☐	☐

Exercise 2: Plane groups

Show that Graphene and the two wallpapers below belong to the same plane group symmetry p6mm. To demonstrate this, use the unit cell below (upper left hand side) on which all symmetry operations are indicated. Demonstrate the presence of the rotation axis, glide planes, mirror planes



Exercise 3: Point groups in 3D



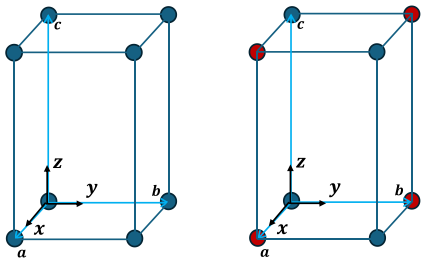
3a. We consider the tetragonal primitive lattice shown on the schematic.

This motif of a rectangular parallelepiped has a point group symmetry noted with: $4/m2/m2/m$. This means that there is a series of operation symmetries that leaves it unchanged, and notably an axis with a 4-fold symmetry, a mirror symmetry perpendicular to this axis, and several similar configuration with two-fold symmetry axis.

(i) Along which axis is the 4-fold symmetry?

(ii) Which are the axis of two 2-fold symmetry?

3b. We consider now the crystal associated with the tetragonal structure



(i) The tetragonal structure, with one atom per motif as shown in the schematic to the left. What is its Space group ?

(ii) We consider a configuration where two atoms (blue and red) are part of the crystal as shown on the schematic to the right.

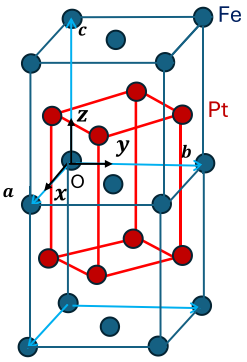
a. Is the 4-fold symmetry conserved ?

(iii) How about the mirror symmetry of the plane perpendicular to the 4-fold axis symmetry ?

Exercise 4: Iron Platinum

Iron-Platinum is a magnetic material that crystalizes in the structure shown. In this structure, we suppose that the Iron atoms sits at the corner of a cube of edge a, as well as at the center of the top and bottom cube faces. Pt atoms sits at the center of the 4 other faces.

The crystal can be formed by translating this cube along the **a**, **b** and **c** orthogonal vectors. On the schematic, two cubes are represented.



4a. What is the chemical structure of this material ?

4b. Show that the crystal structure is actually tetragonal primitive, and find its lattice parameters as a function of a.

4c. Would the symmetries found for the tetragonal structure in questions 2b also be present for this material?

4d. What would you expect its space group to be?