

Read the questions carefully. Answer the questions in the spaces provided on the question sheets. If you run out of room for an answer, continue on the back of the page.

Name and student number: _____

Good luck!

Question 1: **Wulff construction**..... 12 points

Consider the graphene lattice shown in Figure 1 below.

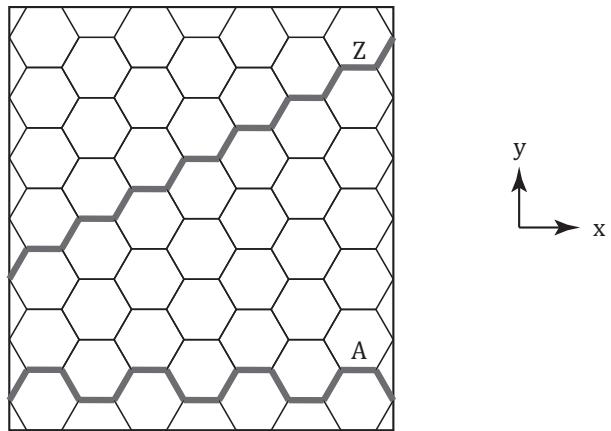


Figure 1: Geometry of a graphene sheet. Zigzag (Z) and armchair (A) directions indicated by a thick gray line. Orientation of x and y axes as indicated.

(a) (2 points) How many equivalent armchair directions are there in graphene? How many equivalent zigzag directions?

(b) (10 points) Assume that the energies of the zigzag and armchair edges are $\gamma_Z = 1.2$ eV and $\gamma_A = 1.0$ eV, respectively. All other edge terminations have a much larger energy. Use the Wulff construction to predict the equilibrium structure of a graphene flake.

Question 2: **Miller indices** 8 points

Consider the crystals shown in Figure 2 below.

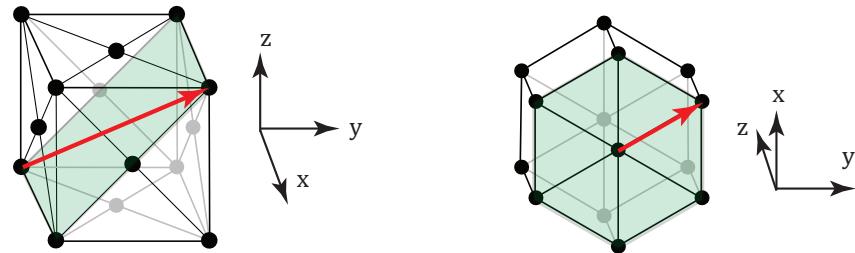


Figure 2: Crystals belonging to the face-centered cubic (left) and hexagonal class (right), respectively.

(a) (8 points) Give the Miller indices of the planes indicated in green and of the arrows indicated in red in Figure 2. Use the axes as indicated in the figure.

Question 3: Angle Resolved Photo Electron Spectroscopy 21 points

(a) (8 points) Give two strong and two weak points of STM and ARPES.

(b) (13 points) In ARPES experiments, the kinetic energy of the photo emitted electrons is given by:

$$E_{kin} = \frac{\hbar^2 k_{\parallel}^2}{2m} \cdot \frac{1}{\sin^2 \theta} \quad (1)$$

Here, \hbar and m are the reduced Planck constant and electron mass, respectively (with values $1.05 \times 10^{-34} \text{ m}^2 \text{ kg s}^{-1}$ and $9.11 \times 10^{-31} \text{ kg}$). Below is a projection of the graphene band structure onto the high symmetry directions of the 2D Brillouin zone. The work function of graphene is 5.11 eV. The coordinates of the K and M points are: $(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a})$, and $(\frac{2\pi}{3a}, 0)$, respectively. a is the C-C bond length (1.42 Å). When performing an ARPES experiment on graphene with a Helium discharge lamp ($h\nu = 21.2 \text{ eV}$), under what angles do you expect to detect electrons coming from the K , M and Γ points?

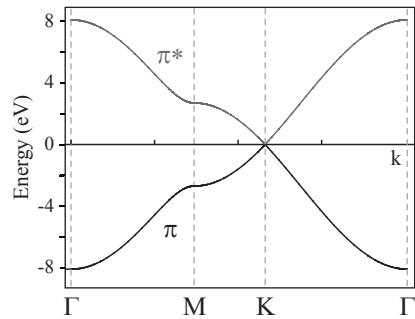


Figure 3: Band structure of graphene along high symmetry directions of the Brillouin zone.

Question 4: **Graphene rolled up to carbon nanotubes** 18 points

Carbon nanotubes (CNTs) can be considered as sheets of graphene rolled into a cylinder. There are various ways in which a sheet can be rolled into a tube, which can be defined using the lattice vector $\mathbf{c}_h = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$, see Figure 2 below. Here, n_1, n_2 are integers and \mathbf{a}_1 and \mathbf{a}_2 are unit vectors of graphene. The CNT is formed by connecting the atoms indicated by the red dots, i.e. the cylinder joint is made along the dotted lines perpendicular to \mathbf{c}_h . The two limiting cases in which the graphene can be rolled are $\theta = 0$ (zigzag direction) and $\theta = \pm 30$ (armchair direction). The resulting tubes are called zigzag and armchair tubes, respectively. All other CNTs are called chiral. You will show that depending on how the sheet is folded, CNTs are either metallic or semiconducting.

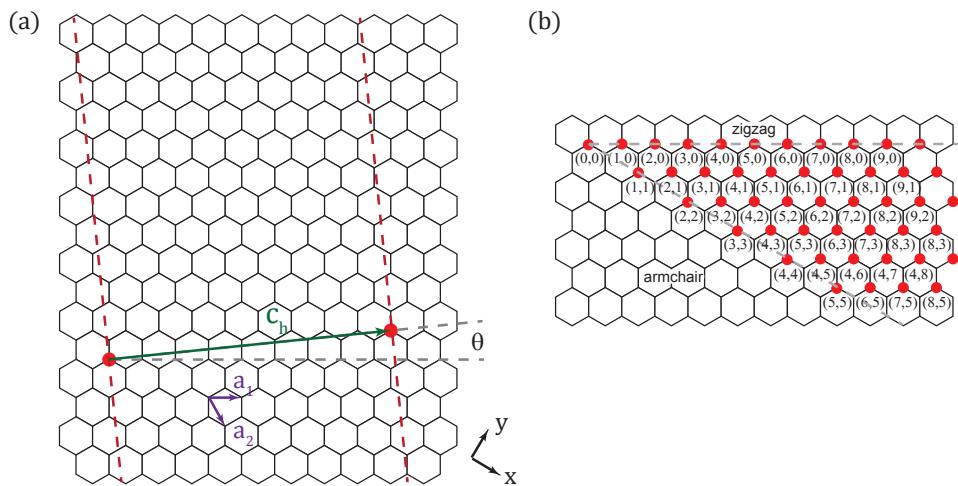


Figure 4: (a) Carbon nanotubes are made by rolling a graphene sheet into a cylinder. CNTs are uniquely defined by the lattice vector \mathbf{c}_h . The chiral angle is denoted by θ , while \mathbf{a}_1 and \mathbf{a}_2 indicate unit vectors of graphene. The x - and y -directions are indicated (same as in exercise 1). (b) Possible vectors for chiral fibers. Armchair and zigzag directions are indicated by dotted lines.

(a) (6 points) Use Blochs' theorem (a wave function in a crystal can change under translation only by a phase factor), together with periodic boundary conditions to show that the following equation holds for carbon nanotubes:

$$\mathbf{c}_h \cdot \mathbf{k} = 2\pi m \quad (2)$$

(b) (2 points) What is needed for a material to be metallic? Which points in the Brillouin zone of graphene fullfill this requirement?

(c) (6 points) The Dirac cones are located at $\left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right)$. Show that the condition for a fiber to be metallic is:

$$2n_1 + n_2 = 3q \quad (3)$$

where q is an integer.

(d) (4 points) Show that this implies that all armchair-CNTs are metallic, while every other third zigzag tube is metallic.