Graphene Nanoribbons

A graphene nanoribbon (GNR) is obtained by patterning a graphene sheet into a narrow ribbon. The electronic properties of a GNR strongly depend on the shape of the edges and the width of the ribbon. The structure of a GNR with so-called *armchair edges* is shown in Fig.1. An armchair GNR is represented by an index N, which denotes the number of carbon atoms of type A (or type B) in a unit cell. The carbon-carbon bond length is $a_0 = 0.142\,\text{nm}$.
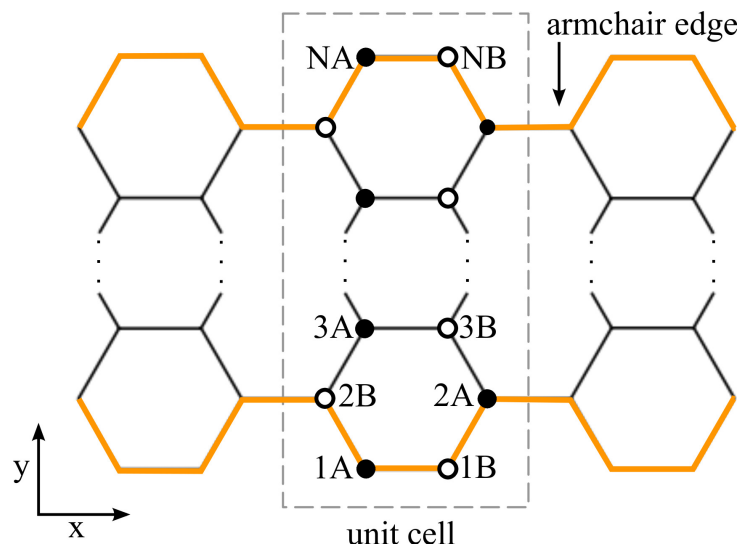

Abbildung 1: The structure of an armchair GNR.

a. Write a function (AGNR_Pos) which calculates the position vectors of the $2N$ carbon atoms in a unit cell of an armchair GNR. Input parameters are the index N and a distance xoff which should be added to the x-coordinate of each atom. The output is the matrix $[\text{Pos}]_{2N \times 2}$ which contains the $2N$ vectors.

b. Write a function (AGNR_Dis) with two input matrices $[\text{Pos1}]_{2N \times 2}$ and $[\text{Pos2}]_{2N \times 2}$ and an output matrix $[\text{Dis}]_{2N \times 2N}$. The function computes the distances Dis[i,j] between atom i in Pos1 and atom j in Pos2.

c. Write a function (AGNR_Ham) with the input matrix $[\text{Dis}]_{2N \times 2N}$ and output matrix $[\text{Ham}]_{2N \times 2N}$. The elements Ham[i,j] indicate the hopping parameter between atom i and atom j. You can assume that the on-site potential is zero ($E_0 = 0$) and that the hopping parameter t is non-zero only for the first nearest neighbors.

$$\text{Ham[i,j]} = \begin{cases} t & \text{if atom i and atom j are nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

The value of the hopping parameter is $t = -2.7\,\text{eV}$.

d. Write a code (`AGNR`) which calculates the Hamiltonian matrix by calling the above functions. First, compute the atomic positions for the central unit cell (`xoff = 0`), of the left unit cell (`xoff = -3a_0`), and of the right unit cell (`xoff = 3a_0`). From the atomic distances within the central unit cell compute the matrix H_{11}. From the distances between the atoms in the left cell and the atoms in the central cell compute the matrix H_{10}. Analogously, compute H_{12}.

Finally, calculate the Hamiltonian $[h(k)]$ by summing the three Hamiltonians with the appropriate phase factors. Use at least 500 discrete k-points in the range $[-\pi/(3a_0), +\pi/(3a_0)]$.

e. For armchair GNRs with $N \in \{6, 7, 8\}$ calculate the eigenvalues with k as a parameter. Plot the eigenvalues as functions of k (dispersion relation).

f. For each GNR, calculate and plot the density of states $D(E)$. One out of two methods can be used:

- Differentiate numerically the dispersion relation $\varepsilon_n(k)$ for each band n to obtain the group velocity v_n.

$$D(E) = \frac{1}{L} \sum_n \sum_{k_\alpha} \delta(E - \varepsilon_n(k_\alpha)) = \frac{1}{\pi\hbar} \sum_n \frac{1}{|v_n(E)|}$$

- Use the original definition of the density of states and replace the δ-function by a Lorentzian function.

$$D(E) = \frac{1}{L} \sum_n \sum_{k_\alpha} \frac{\gamma/2\pi}{(E - \varepsilon_n(k_\alpha))^2 + (\gamma/2)^2}$$

The broadening factor γ has to be chosen carefully.

Your report should be in PDF format and include figures, discussions, and the source codes. If you have questions please contact **kampl@iue.tuwien.ac.at** or **kosina@iue.tuwien.ac.at**. Please upload your report on TUWEL by **June 9, 2017.**