Modeling and simulation methods in nanotechnology. Practical laboratory

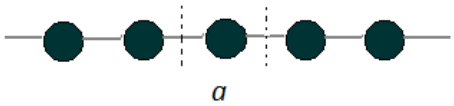
Solving practical tasks in computer laboratory. 6 hours

Practical application of tight-binding method to numerical calculations of energy bands in selected graphene structures.

Task 1.

One-dimensional chain of atoms. Construction of molecular orbital and Hamiltonian matrix.

This is arithmetical task. Let us consider a system as show in the figure:



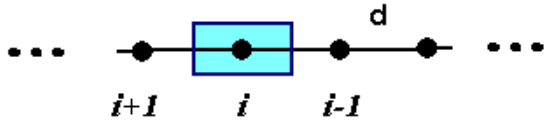
Atoms are represented by Black points and chemical bonds by lines. The lattice constant is assigned as *a.* W assume one (valence) orbital χ per atom . Although χ can depend on three special variables, symbolically we write the dependence only on **x,** since this is the direction of periodicity. We assume N atoms in this chain. χ(x-na) is an orbital situated on *n*-th atom in the chain. We create a molecular (crystal) orbital fulfilling the Bloch theorem, as

$$\phi(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} \chi(x - na)$$

The energy of electron in such a chain (precisely the energy expectation value in a state described by function ϕ , i.e. matrix element of **H** is

$$E = \langle \phi | \mathbf{H} | \phi \rangle .$$

Since each ϕ is a sum of many χ, therefore, applying the nearest neighbors approximation, i.e. assuming that different than zero are only those $\langle \chi_i | \mathbf{H} | \chi_j \rangle$ elements, where j=i and when j differs from I by only one position (the nearest neighbor).



Next, putting $\langle \chi_i | \mathbf{H} | \chi_i \rangle = 0$ (i.e. the energy scaling) we finally get

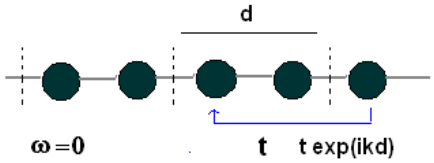
$$E = \langle \chi_0 | \mathbf{H} | \chi_1 \rangle e^{ikd} + \langle \chi_0 | \mathbf{H} | \chi_{-1} \rangle e^{-ikd} = t 2\cos(kd) \quad (1)$$

that means a single band E(k).
Students have to derive the formula (1) and draw E(k) in any graphical tool.

Task 2.

One-dimensional chain as in task.1, but now unit cell contains two atoms.

The aims of this exercise are: (1) derive formula for Hamiltonian matrix elements, (2) understanding that the resulting bands, come out are energetically equivalent to the band obtained in task.1, (3) to show that the bands can be obtained by folding BZ from the task.1.
Now, we have the same chain but the unit cell is defined in a different way.



Now, the dimension of Hamiltonian matrix is 2 (two atoms in a unit cell). Setting diagonal elements equal zero we get

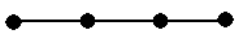
$$H = \begin{bmatrix} 0 & t(1+e^{ikd}) \\ t(1+e^{-ikd}) & 0 \end{bmatrix}$$

The energy spectrum is the same as in task.1, although now built of two bands. It is important to notice the difference in the size of BZ in both cases. Matrix can be diagonalized "by hand" or one can write a code , which will construct H and call appropriate procedure (diagonalization).

Task 3.

Construction of the Hamiltonian matrix for a few-atomic molecule.

For ex ample, „molecule" C_4

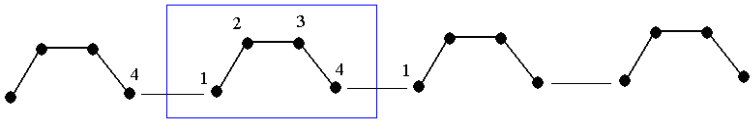


$H_{ii} = 0$, i=1,2,3,4 - as diagonal elements, $H_{12} = H_{21} = H_{23} = H_{32} = H_{34} = H_{43} = t$ [= -2.7 eV] All the others $H_{kl} = 0$; here H doesn't depend on *k*

Task4.

Construction of the Hamiltonian matrix for the simplest (the most narrow) armchair graphene Ribbon.

First, one has to enumerate all the nodes (atoms) in t hunt cell (also separately in the neighbor unit cells).

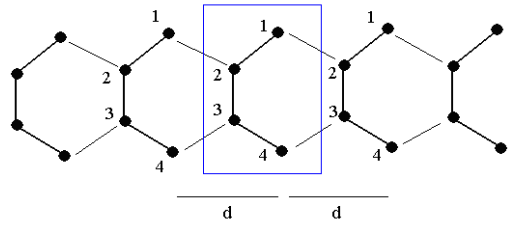


$$H = \begin{bmatrix} 0 & t & 0 & t(e^{-ikd}) \\ t & 0 & t & 0 \\ 0 & t & 0 & t \\ t(e^{ikd}) & 0 & t & 0 \end{bmatrix}$$

Task 5.

Construction of the Hamiltonian matrix for the simplest (the most narrow) zigzag graphene Ribbon.

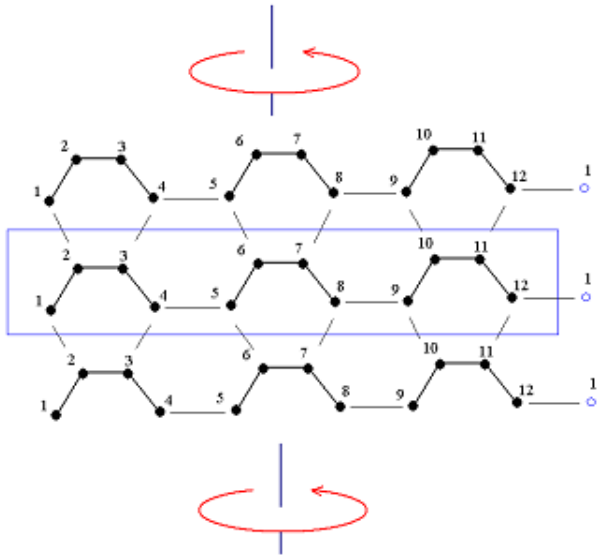
First, one has to enumerate all the nodes (atoms) in t hunt cell (also separately in the neighbor unit cells).



$$H = \begin{bmatrix} 0 & t(1+e^{ikd}) & 0 & 0 \\ t(1+e^{-ikd}) & 0 & t & 0 \\ 0 & t & 0 & t(1+e^{-ikd}) \\ 0 & 0 & t(1+e^{ikd}) & 0 \end{bmatrix}$$

Task 6.

Construction of the Hamiltonian matrix for carbon nanotube (3,3)



And matrix H (dimension = 12)

$$
\begin{bmatrix}
0 & t(1+e^{ikd}) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t \\
t(1+e^{-ikd}) & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & t & 0 & t(1+e^{-ikd}) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & t(1+e^{ikd}) & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & t & 0 & t(1+e^{ikd}) & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & t(1+e^{-ikd}) & 0 & t & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & t & 0 & t(1+e^{-ikd}) & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & t(1+e^{ikd}) & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & t & & & & \\
 & & & & & & & & etc... & & & \\
 & & & & & & & & & & &
\end{bmatrix}
$$

Final classification task.

Construction and execution of a computer code for calculating energy structure of any graphene systems, periodic and non-periodic ones.

General structure of the code:

- Determination of the number of nodes atoms) in the unit cell, N= dimH,
- Definition of bonds (connections) within a given unit cell; determination of elements, which are H_{ij} = t,
- Definition of connections (bonds) between atoms belonging to neighbor unit cells, (te(ik), or t[1+eik]),
- Loop over all k values (in BZ)
  - diagonalization of H for each *k*, using any appropriate method, depending on the programming language or package and platform chosen,
- Allow for different strengths of Bond (t) in different regions,
- Allow for unit cell modification by adding or removing atoms,
- Write the results (energy bands) down to a file
- Make diagrams of the calculated energy bands.

Students can chose any language or computational package they wish Fortran, C, C++, Csharp, Matlab, Phyton, etc..). They can utilize ready-to-use libraries and procedures for diagonalization of complex, hermitian matrices.

For classification, students must demonstrate they now their codes in detail. They must execute the code for a system chosen by the teacher (e.g., carbon tube (6,6), carbon tube (5,0), graphene zigzag Ribbon with one edge modified by different number of Klein nodes).