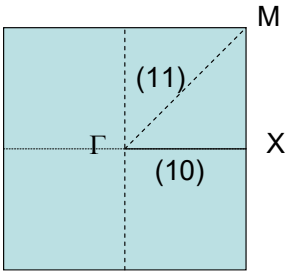
Homework Assignment #2
Due Wednesday, March 5, 11:59 pm



Problem 1: Using the tight-binding model, compute the energy band formed by atomic *s*-orbitals in a square lattice of constant a (Brillouin zone is depicted to your left), with a single atom basis. Use $\varepsilon_{\vec{q}} = \varepsilon_s - \beta - \gamma \sum_{\substack{nearest \\ neighbors}} \exp(i\vec{q}\cdot\vec{R})$, where $\varepsilon_S, \beta, \gamma$ (the s-level atomic energy and the overlap integrals, respectively) are considered to be known.

a) Plot the energy band ($\varepsilon_{\vec{q}}$ vs $\vec{q}$) in 3D.

b) Plot the energy vs $\vec{q}$ along certain directions: going from M to Γ, then from Γ to X, then from X back to M. (This will be a 2D plot.)

Problem 2: Using the tight-binding (LCAO) approach, compute the energy band formed by atomic *s*-orbitals in an fcc lattice with a monoatomic basis. Plot the energy vs $\vec{q}$ along L—Γ—X—U— Γ (Note: Find coordinates of U and L in Ashcroft and Mermin).

Problem 3: Redo the "Mock 1D NaCl" problem that we did in class. A 1D chain consists of alternating Na and Cl atoms, with the spacing between Na and Cl them being a. If Na contributes its *s* orbital (energy *E*s) and Cl contributes its p_x orbital (energy *E*p) to the formation of this fictitious crystal, with the magnitude of the overlap integral denoted as *E*sp, answer the following:

a) What is the lattice period?

b) How many atoms are in the basis?

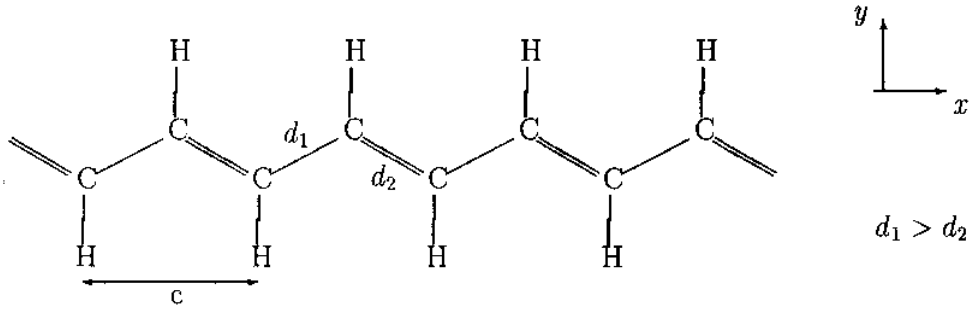
c) How many bands will form?

d) Calculate and graph the energy dispersions for all the bands across the Brillouin zone.

Problem 4: One of the simplest conjugated polymers is polyacetylene, whose structure is shown below. The double bonds are known to be slightly shorter than the single bonds (this phenomenon is called *dimerization*). Polyacetylene can be modeled as a solid with a one-dimensional Bravais lattice along the *x*-axis.

a) What is the lattice period (from the picture)?

b) What are the atoms that constitute the basis? (The basis—a periodically repeated unit—is called a *monomer* in the case of polymeric chains).



The hydrogen atom contributes to bonding with one electron in its 1s orbital, while C is in group 4, and contributes with 4 electrons distributed over its 2s and 2p orbitals (a total of 4 orbitals).

c) How many bands will form?

When the chain is formed, carbon's 2s orbital and two of its three 2p orbitals form the bonds C-C and C-H that are located in the plane of the picture (the so-called σ -bonds). In addition, each of the carbon atoms has an extra p_z orbital, perpendicular to the plane of the paper, which overlap sideways and form the weaker π bond.

d) Assuming that two of the bands are formed by the carbon p_z orbitals alone, use a simple nearest-neighbor tight-binding model to calculate the bandstructure of these two bands. Also, plot the calculated bandstructure within the first Brillouin zone.

In your calculation, assume the energy E_p of the atomic p-level is known, and utilize the simplified tight-binding formulas

$$\left(E_{\vec{q}} - E_p\right) b^{(i)} = \sum_j \sum_{\substack{\vec{R} \text{ over nearest} \\ \text{neighbors}}} \left\langle \Phi^{(i)}_{p_z} \middle| \Delta U \middle| \Phi^{(j)}_{p_z, \vec{R}+\vec{d}_j} \right\rangle e^{i\vec{q}\left(\vec{R}+\vec{d}_j\right)} b^{(j)} \ ,$$

where *i*,*j* number the carbon atoms in the basis (those whose p_z orbitals you are mixing).

Neglect the matrix elements of ΔU on the same site and retain only

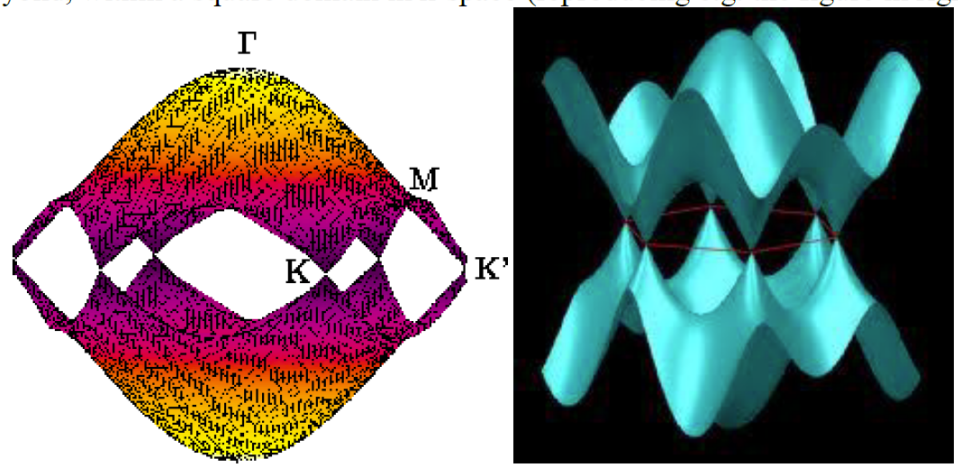
$$\left\langle \Phi^{(i)}_{p_z} \middle| \Delta U \middle| \Phi^{(j)}_{p_z, R+d_j} \right\rangle = \gamma_1 \quad \text{if carbon atoms } i \text{ and } j \text{ are joined by a single bond}$$

$$\left\langle \Phi^{(i)}_{p_z} \middle| \Delta U \middle| \Phi^{(j)}_{p_z, R+d_j} \right\rangle = \gamma_2 \quad \text{if carbon atoms } i \text{ and } j \text{ are joined by a double bond}$$

Note: In the final expression, the angles between the bonds and the *x*-axis are not needed – the only distance appearing will be the Bravais lattice constant.

Problem 5

a) Plot the bandstructure throughout the 1st Brillouin zone (reproducing e.g figure in left panel) and beyond, within a square domain in k-space (reproducing e.g. the figure in right panel)



b) Plot the band structure along the K—Γ—M—K directions, such as in Fig 2 of this paper. There are plenty of resources for calculating the band structure of graphene on the web, such as this writeup.

https://qtts.engr.wisc.edu/wp-content/uploads/sites/1194/2020/08/SuleJAP2012.pdf

http://www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf