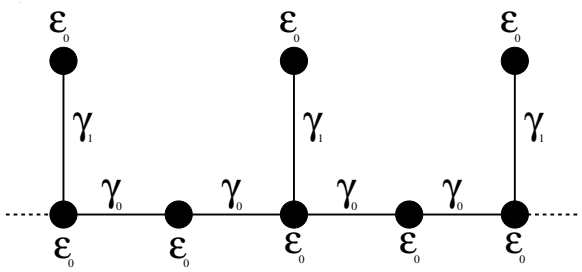
**5001 Electronic Structure: Assignment 1**

1. Consider a linear chain of H atoms with the following geometry.



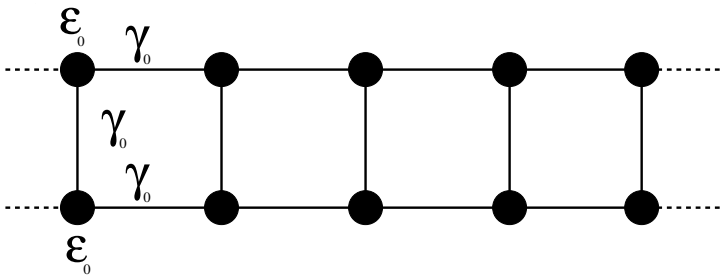

Suppose that the distance between the H atoms is different within the structure. In this case there is the possibility to have two different hopping integral $\gamma$ as indicated in figure.

   (a) Demonstrate that the band structure has two main components: a standard hydrogenic-like band plus a dispersionless band.

   (b) Calculate the band structure in the limit of $\gamma_1 \to 0$ and discuss the result.

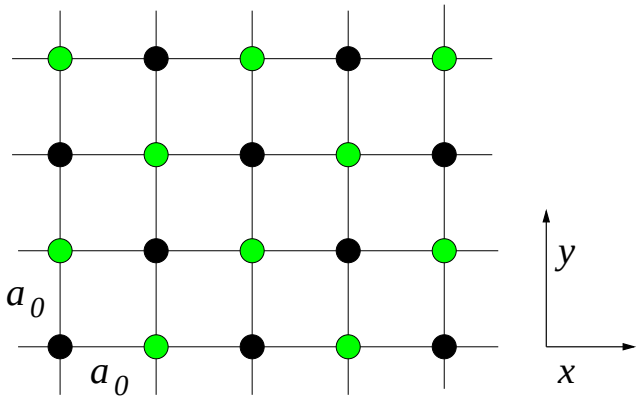
   (c) Calculate the band structure in the limit of $\gamma_0 \to 0$ and discuss the result.

2. Consider a two dimensional square lattice with lattice constant $a_0$ made from Li atoms, and assume to cut an infinite slab with two atoms in the cross section (see figure).




Describe the system using a $2s$ nearest neighbour orthogonal tight-binding model with on-site energy $\epsilon_0$ and hopping integral $\gamma_0$ ($\gamma_0 < 0$). Starting from the infinite 2D square lattice calculate the band structure of the slab.

3. Consider the following 2D lattice (2D rocksalt) formed by alternating Na (black circles) and Cl (gray circles) atoms.



Calculate the bandstructure equation assuming an orthogonal nearest neighbors tight-binding model with one orbital per atom (respectively $|\mathrm{Na}\rangle$ and $|\mathrm{Cl}\rangle$) and the following matrix elements:

$$\langle \mathrm{Na}|H|\mathrm{Na}\rangle = \epsilon_N$$

$$\langle \mathrm{Cl}|H|\mathrm{Cl}\rangle = \epsilon_C$$

$$\langle \mathrm{Na}|H|\mathrm{Cl}\rangle = \langle \mathrm{Cl}|H|\mathrm{Na}\rangle = \gamma$$

Draw schematically the band structure along the following direction $(k_x, k_y)$:

$$(0,0) \rightarrow (0, \pi/a_0) \rightarrow (\pi/a_0, \pi/a_0) \rightarrow (0,0) \rightarrow (\pi/a_0, 0)$$

assuming $\epsilon_C$=0 eV, $\epsilon_N$=6 eV, $\gamma$=-1 eV.