ECE 495N

Fundamentals of Nanoelectronics

Fall 2008

Instructor: Supriyo Datta
Purdue University

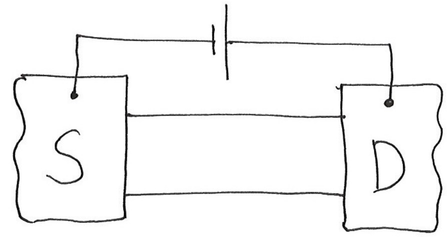
Lecture: 21
Title: Graphene Bandstructures
Date: October 20, 2008

Video Lectures posted at:
https://www.nanohub.org/resources/5346/

Class notes taken by: Panagopoulos Georgios
Purdue University

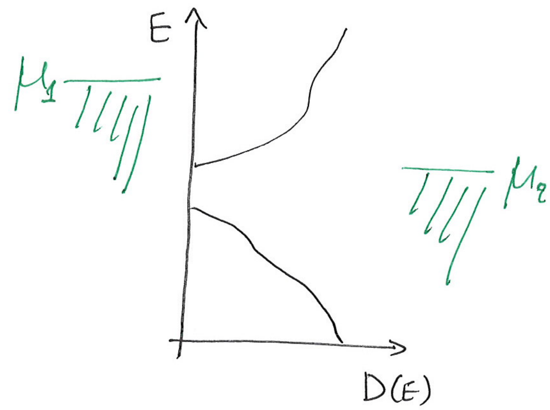
Graphene Bandstructures | Lecture 21 | Oct, 20, 2008

$$E\,\Phi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U\right)\Phi$$



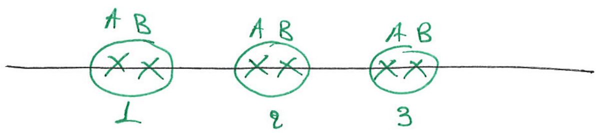
$$E\{\phi\} = \overbrace{[H]}^{N_b\times N_b}\{\phi\}$$

$$E\{\phi_n\} = \sum_m [H_{nm}]\,\phi_m$$



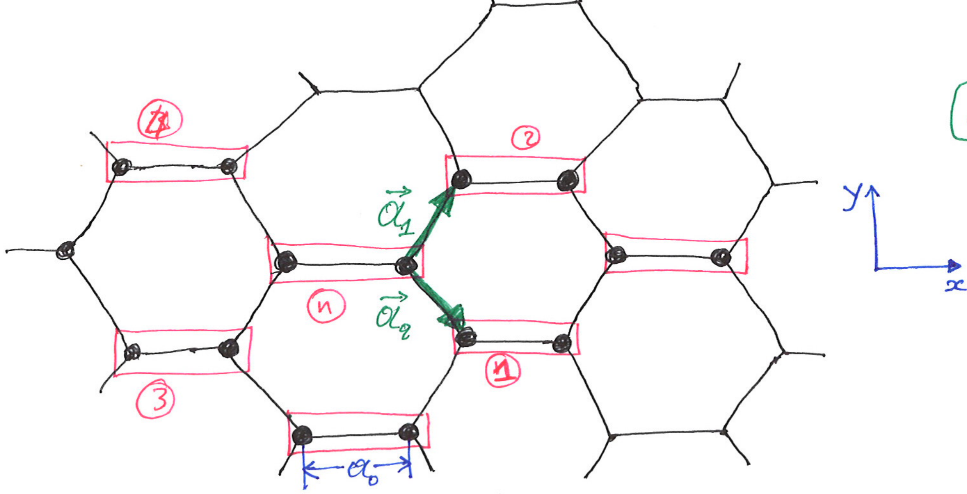
$$\begin{Bmatrix}\phi_1\\ \phi_2\end{Bmatrix} \sim \{\phi_n\} = \{\phi_0\}\,e^{i\vec{k}\cdot\vec{d}_n}$$

$$\underbrace{[h]}_{b\times b}\{\phi_0\} = E\{\phi_0\}$$



$$\boxed{h(\vec{k}) = \sum_m [H_{nm}]\,e^{i\vec{k}\cdot(\vec{d}_m-\vec{d}_n)}}$$

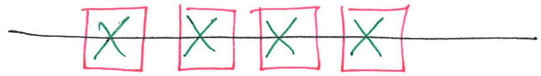
Graphene

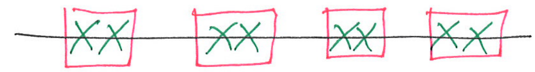


$1s^2$

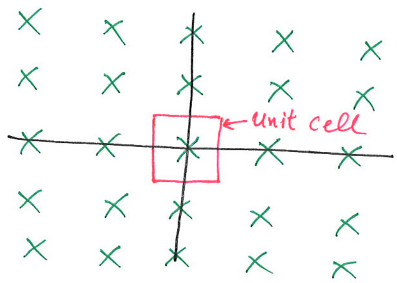
$\underbrace{2s^2\ 2p_x^2\ 2p_y}\ \ 2p_z$

Two disjoint groups





If you define two vectors $\vec{a}_1$ and $\vec{a}_2$ and you are able to write the position of every other atom as a combination of $m\vec{a}_1 + n a_2$, m, n integer then we can show that this define a unit cell.



For the graphene the vectors $\vec{a}_1$, $\vec{a}_2$ are:

$$\vec{a}_1 = \hat{x}\,\frac{3a_0}{2} + \hat{y}\,\frac{\sqrt{3}\,a_0}{2} \quad \text{and} \quad \vec{a}_2 = \hat{x}\,\frac{3a_0}{2} - \hat{y}\,\frac{\sqrt{3}\,a_0}{2}$$

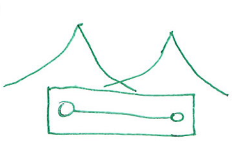
Let's now to form the matrix $h(\vec{k})$

$$[h(\vec{k})] = \begin{array}{cc} n & \begin{array}{cc} n\;\; A & \quad B \end{array} \\ \begin{array}{c} A \\ B \end{array} & \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix} \end{array}$$

connection to the nearest neighbor

$$+ \begin{array}{cc} n & \begin{array}{cc} 1\;\; A & \quad B \end{array} \\ \begin{array}{c} A \\ B \end{array} & \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix} \end{array} e^{i\vec{k}\cdot\vec{a}_1} + \begin{array}{cc} n & \begin{array}{cc} 2\;\; A & \quad B \end{array} \\ \begin{array}{c} A \\ B \end{array} & \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix} \end{array} e^{i\vec{k}\cdot\vec{a}_2}$$

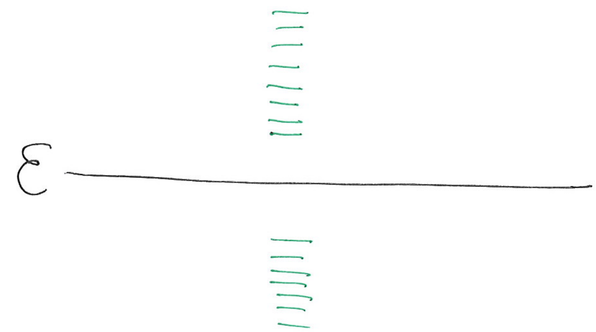
$$+ \begin{array}{cc} n & \begin{array}{cc} 3\;\; A & \quad B \end{array} \\ \begin{array}{c} A \\ B \end{array} & \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} \end{array} e^{-i\vec{k}\cdot\vec{a}_1} + \begin{array}{cc} n & \begin{array}{cc} 4\;\; A & \quad B \end{array} \\ \begin{array}{c} A \\ B \end{array} & \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} \end{array} e^{-i\vec{k}\vec{a}_2}$$

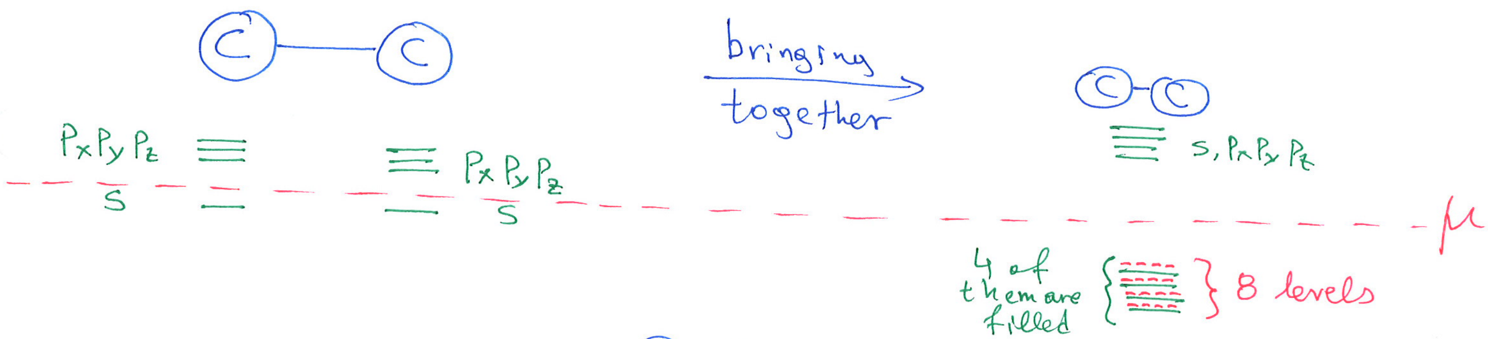


$$\Rightarrow h(\vec{k}) = \left[\begin{array}{c|c} \varepsilon & t\left(1+e^{-i\vec{k}\cdot\vec{a}_1}+e^{-i\vec{k}\cdot\vec{a}_2}\right) \\ \hline t\left(1+e^{+i\vec{k}\cdot\vec{a}_1}+e^{+i\vec{k}\cdot\vec{a}_2}\right) & \varepsilon \end{array}\right]$$

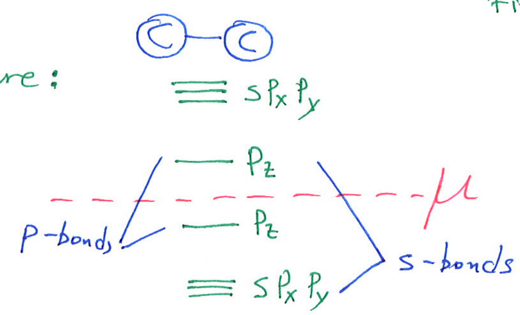
$$= \begin{bmatrix} \varepsilon & h_0 \\ h_0^* & \varepsilon \end{bmatrix} \quad \text{where } h_0 = t\left(1+e^{-i\vec{k}\cdot\vec{a}_1}+e^{-i\vec{k}\cdot\vec{a}_2}\right)$$

eigenvalues: $\varepsilon \pm |h_0|$

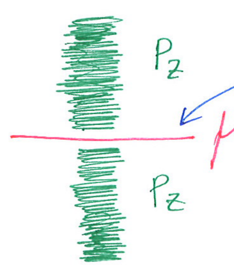




More correctly the levels are:



In a big lattice we have:



if we doped the graphene then we will move the μ up and up