Electronic Structure of Graphene

Hasdeo

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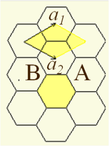
Outline

Prosedur Mendapatkan Dispersi Energi

1. Tentukan
   1. unit cell dan unit vektor $\mathbf{a}_i$,
   2. tentukan koordinat atom pada unit cell
   3. dan tentukan jumlah n orbital atom yang diperhitungkan
2. Carilah Brillouin zone dan reciprocal lattice vector $\mathbf{b}_i$
3. Hitung $\mathscr{H}_{ij}(\mathbf{k})$ dan $S_{ij}(\mathbf{k})$
4. Selesaikan persamaan sekular, dapatkan $E_i(\mathbf{k})$ dan $C_{ij}(\mathbf{k})$.

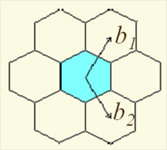
Graphene unit cell



Diketahui:

1. 2 atom per unit cell,
   1. unit vektor
   $$\mathbf{a}_1 = \left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) a,\ \mathbf{a}_2 = \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) a$$
   2. koordiat atom
   $$\mathbf{R}_l^{B\to A} = \left(\frac{1}{\sqrt{3}}, 0\right) a,\ \left(-\frac{1}{2\sqrt{3}}, \frac{1}{2}\right) a,\ \left(-\frac{1}{2\sqrt{3}}, -\frac{1}{2}\right) a$$
   3. hanya perhitungkan π orbital

1. Brillouin Zone



1. Vektor kisi resiprok

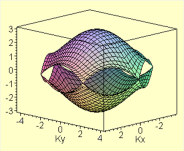
$$\mathbf{b}_1 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \frac{4\pi}{\sqrt{3}a}, \ \mathbf{b}_2 = \left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right) \frac{4\pi}{\sqrt{3}a}$$

1. $H_{AA} = H_{BB} = 0,$
   $H_{AB} = H_{BA}^{*} = -t\left(e^{ik_x a/\sqrt{3}} + 2e^{-ik_x a/2\sqrt{3}} \cos\frac{k_y a}{2}\right)$
2. Secular Equation

$$\begin{aligned} \det\left[H - E_k S\right] &= 0 \\ \det\begin{bmatrix} H_{AA} - E_k & H_{AB} \\ H_{AB}^{*} & H_{BB} - E_k \end{bmatrix} &= 0 \end{aligned}$$

$$E_k = \sqrt{\left|H_{AB}\right|^2} = \pm t\sqrt{1 + 4\cos\frac{k_y a}{2}\cos\frac{\sqrt{3}k_x a}{2} + 4\cos^2\frac{k_y a}{2}}$$

3. Energy Dispersion



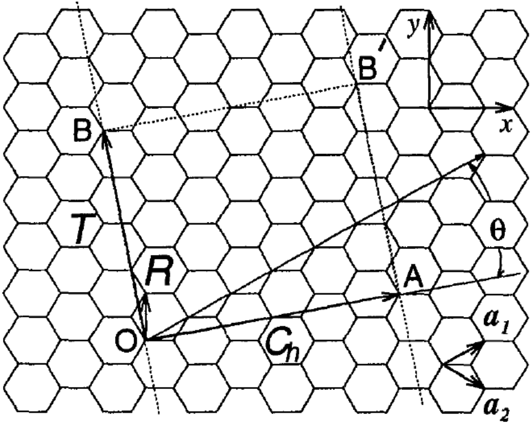
Lapack Programming

Saatnya belajar Lapack

σ and π band of Graphene

Pelajari buku Physical *Properties of Carbon Nanotube* Sect. 2.3.2 dan dapatkan gambar 2.8

SWNT unit cell



SWNT geometry properties

Table 3.3: Parameters for Carbon Nanotubes.[a]

symbol	name	formula	value
a	length of unit vector	$a = \sqrt{3}a_{C-C} = 2.49$ Å,	$a_{C-C} = 1.44$ Å
$\boldsymbol{a}_1, \boldsymbol{a}_2$	unit vectors	$\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)a, \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)a$	x, y coordinate
$\boldsymbol{b}_1, \boldsymbol{b}_2$	reciprocal lattice vectors	$\left(\frac{1}{\sqrt{3}}, 1\right)\frac{2\pi}{a}, \left(\frac{1}{\sqrt{3}}, -1\right)\frac{2\pi}{a}$	x, y coordinate
$\boldsymbol{C}_h$	chiral vector	$\boldsymbol{C}_h = n\boldsymbol{a}_1 + m\boldsymbol{a}_2 \equiv (n, m)$,	$(0 \le \lvert m\rvert \le n)$
L	length of $\boldsymbol{C}_h$	$L = \lvert\boldsymbol{C}_h\rvert = a\sqrt{n^2 + m^2 + nm}$	
d_t	diameter	$d_t = L/\pi$	
θ	chiral angle	$\sin\theta = \frac{\sqrt{3}m}{2\sqrt{n^2 + m^2 + nm}}$	$0 \le \lvert\theta\rvert \le \frac{\pi}{6}$
		$\cos\theta = \frac{2n + m}{2\sqrt{n^2 + m^2 + nm}}$,	$\tan\theta = \frac{\sqrt{3}m}{2n + m}$
d	$\gcd(n,m)$[b]		
d_R	$\gcd(2n + m, 2m + n)$[b]	$d_R = \begin{cases} d & \text{if } (n-m) \text{ is multiple of } 3d \\ 3d & \text{if } (n-m) \text{ is not multiple of } 3d \end{cases}$	
$\boldsymbol{T}$	translational vector	$\boldsymbol{T} = t_1\boldsymbol{a}_1 + t_2\boldsymbol{a}_2 \equiv (t_1, t_2)$	$\gcd(t_1, t_2) = 1$[b]
		$t_1 = \frac{2m + n}{d_R},\ t_2 = -\frac{2n + m}{d_R}$	
T	length of $\boldsymbol{T}$	$T = \lvert\boldsymbol{T}\rvert = \frac{\sqrt{3}L}{d_R}$	
N	Number of hexagons in the nanotube unit cell.	$N = \frac{2(n^2 + m^2 + nm)}{d_R}$	
$\boldsymbol{R}$	symmetry vector	$\boldsymbol{R} = p\boldsymbol{a}_1 + q\boldsymbol{a}_2 \equiv (p, q)$	$\gcd(p, q) = 1$[b]
		$t_1 q - t_2 p = 1,\ (0 < mp - nq \le N)$	
τ	pitch of $\boldsymbol{R}$	$\tau = \frac{(mp - nq)T}{N} = \frac{MT}{N}$	
ψ	rotation angle of $\boldsymbol{R}$	$\psi = \frac{2\pi}{N}$	in radians
M	number of $\boldsymbol{T}$ in $N\boldsymbol{R}$.	$N\boldsymbol{R} = \boldsymbol{C}_h + M\boldsymbol{T}$	

[a] In this table n, m, t_1, t_2, p, q are integers and d, d_R N and M are integer functions of these integers.

[b] $\gcd(n, m)$ denotes the greatest common divisor of the two integers n and m.