GRAFEN, ENERJİ BAND YAPISI

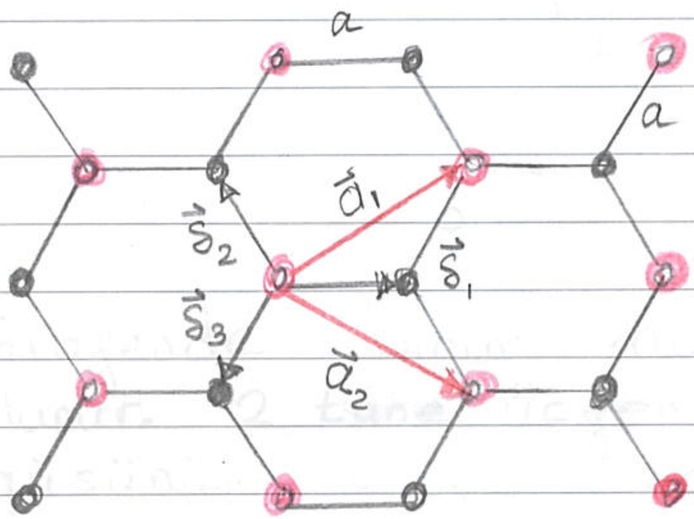
Karbon atomu: $1s^2\ 2s^2\ 2p^2$

Karbonun 4 valens elektronunun 3 tanesi kovalent bağ oluşturmak için kullanılır. Geriye kalan tek elektronun enerji band yapısı hesaplanacaktır.

Örgü yapısı: Bal peteği (Honecomb)

Örgü parametreleri: $\vec{a}_1 = \frac{a}{2}(3, \sqrt{3})$

$\vec{a}_2 = \frac{a}{2}(3, -\sqrt{3})$



En yakın komşu uzaklıkları:

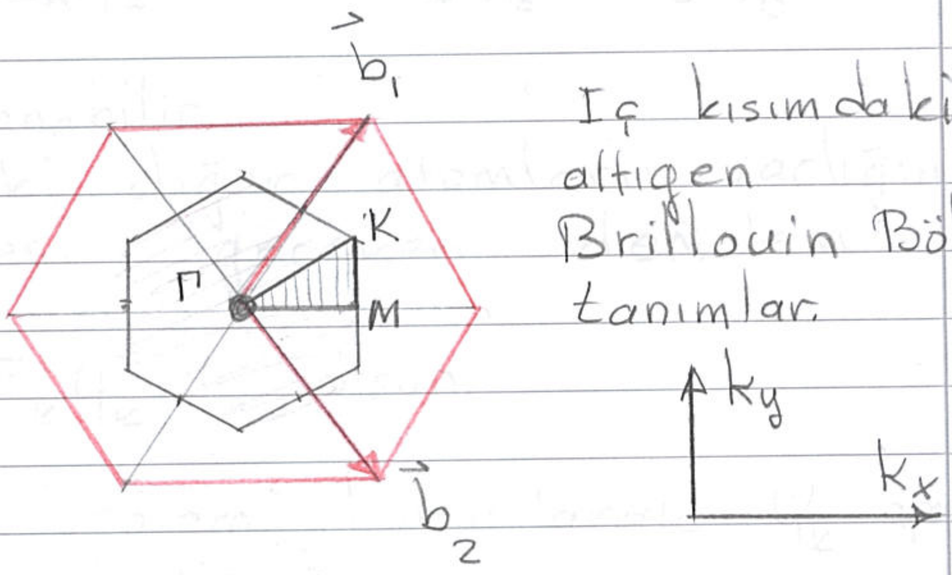
$$\vec{\delta}_1 = a(1,0) = \frac{1}{3}(\vec{a}_1 + \vec{a}_2)$$

$$\vec{\delta}_2 = \frac{a}{2}(-1, \sqrt{3}) = \vec{\delta}_1 - \vec{a}_2 = \frac{1}{3}(\vec{a}_1 - 2\vec{a}_2)$$

$$\vec{\delta}_3 = \frac{a}{2}(-1, -\sqrt{3}) = \vec{\delta}_1 - \vec{a}_1 = \frac{1}{3}(\vec{a}_2 - 2\vec{a}_1)$$

Ters örgü :

$$\vec{b}_1 = \frac{2\pi}{a}(1, \sqrt{3}) \qquad \vec{b}_2 = \frac{2\pi}{a}(1 -\sqrt{3})$$



Iç kısımdaki altıgen Brillouin Bölge tanımlar.

Grafende birim hücrede 2 atom bulunur. 2 tane üçgen Bravais örgüsünün iç içe girmiş biçimidir.

Komşu atomlara örgü vektörü $\vec{R}$ ile ulaşılamaz. Bunun için ek paramet gereklidir $(\vec{\delta}_1, \vec{\delta}_2, \vec{\delta}_3)$.

$$|\vec{\delta}_1| = |\vec{\delta}_2| = |\vec{\delta}_3| = a$$

Birim hücrede her bir atoma ait dalga fonksiyonları diğer atomların yokluğunda atomik dalga fonksiyonu olarak ϕ_A, ϕ_B

$$H_A \phi_A = E_A \phi_A \qquad H_B \phi_B = E_B \phi_B \qquad (E_A = \ldots$$

tanımlanabilir.

Örgüdeki diğer atomların varlığında çözülmesi gereken denklem

$$H \psi_k = E_k \psi_k$$ olsun.

Bloch teoremi kullanılarak ψ_k aşağıda gibi yazılabilir:

$$\psi_k(\vec{r}) = b_1 \sum_{R_i} e^{i\vec{k}\cdot\vec{R}_i} \phi_A(\vec{r} - \vec{R}_i) + b_2 \sum_{R_i} e^{i\vec{k}\cdot\vec{R}_i} \phi_B(\vec{r} - (\vec{\delta}_1 + \vec{R}_i))$$

Bir önceki örnekte gösterildiği gibi enerjiyi verecek determinant

$$\det \begin{bmatrix} H_{11} - E_k S_{11} & H_{12} - E_k S_{12} \\ H_{21} - E_k S_{21} & H_{22} - E_k S_{22} \end{bmatrix} = 0$$

olmalıdır.

$$H_{11} = N \sum_{R_m} e^{i\vec{k}\cdot\vec{R}_m} \langle \phi_A(\vec{r}) | H | \phi_A(\vec{r} - \vec{R}_m) \rangle$$

$$H_{22} = N \sum_{R_m} e^{i\vec{k}\cdot\vec{R}_m} \langle \phi_B(\vec{r} - \vec{\delta}_1) | H | \phi_B(\vec{r} - (\vec{\delta}_1 + R_m)) \rangle$$

$$H_{12} = N \sum_{R_m} e^{i\vec{k}\cdot\vec{R}_m} \langle \phi_A(\vec{r}) | H | \phi_B(\vec{r} - (\vec{\delta}_1 + \vec{R}_m)) \rangle$$

$$H_{21} = N \sum_{R_m} e^{i\vec{k}\cdot\vec{R}_m} \langle \phi_B(\vec{r} - (\vec{\delta}_1 - R_m)) | H | \phi_A(\vec{r}) \rangle$$

$$S_{11} = N \sum_{R_m} e^{i\vec{k}\cdot\vec{R}_m} \langle \phi_A(\vec{r}) | \phi_A(\vec{r} - R_m) \rangle$$

$$= N(1 + \text{ihmal})$$

$$S_{22} = N \sum_{R_m} e^{i\vec{k}\cdot\vec{R}_m} \langle \phi_B(\vec{r} - \vec{\delta}_1) | \phi_B(\vec{r} - (\vec{\delta}_1 + R$$

$$= N(1 + \text{ihmal})$$

S ATAG

$$S_{12} = N \sum_{R_m} e^{i\vec{k}\cdot\vec{R}_m} \langle \phi_A(\vec{r}) | \phi_B(\vec{r} - (\vec{\delta}_1 + R_m)) \rangle$$

$$S_{21} = N \sum_{R_m} e^{i\vec{k}\cdot\vec{R}_m} \langle \phi_B(\vec{r} - (\vec{\delta}_1 - \vec{R}_m)) | \phi_A(\vec{r}) \rangle$$

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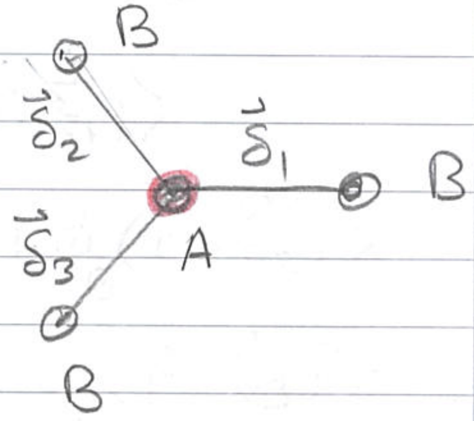
İlk Yaklaşım: Sadece En Yakın Komşu Etkileşmesi



$$\vec{\delta}_1 = \vec{\delta}_1 + \vec{R}_m \qquad \boxed{\vec{R}_m = 0}$$

$$\vec{\delta}_2 = \vec{\delta}_1 + \vec{R}_m \qquad \vec{R}_m = m_1 \vec{a}_1 + m_2 \vec{a}_2$$

$$\boxed{\vec{\delta}_2 = \vec{\delta}_1 - \vec{a}_2} \qquad \boxed{\vec{R}_m = -\vec{a}_2} \qquad m_2 = -1$$

$$\vec{\delta}_3 = \vec{\delta}_1 + \vec{R}_m$$

$$\boxed{\vec{\delta}_3 = \vec{\delta}_1 - \vec{a}_1} \qquad \boxed{\vec{R}_m = -\vec{a}_1} \qquad m_1 = -1$$

——— o ———

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$$\vec{\delta}_1 = \vec{\delta}_1 - \vec{R}_m \qquad \vec{\delta}_1 = \vec{\delta}_1 \qquad \boxed{\vec{R}_m = 0}$$

$$\vec{\delta}_2 = \vec{\delta}_1 - \vec{a}_2 \qquad \boxed{\vec{R}_m = \vec{a}_2}$$

$$\vec{\delta}_3 = \vec{\delta}_1 - \vec{a}_1 \qquad \boxed{\vec{R}_m = \vec{a}_1}$$

$$H_{11} = E_A \qquad H_{22} = E_B$$

$$H_{12} = \langle \phi_A(\vec{r}) | H | \phi_B(\vec{r} - \vec{\delta}_1) \rangle + e^{-i\vec{k}\cdot\vec{a}_2} \langle \phi_A(\vec{r}) | H | \phi_B(\vec{r} - \vec{\delta}_2) \rangle + e^{-i\vec{k}\cdot\vec{a}_1} \langle \phi_A(\vec{r}) | H | \phi_B(\vec{r} - \vec{\delta}_3) \rangle$$

$$H_{21} = \langle \phi_B(\vec{r} - \vec{\delta}_1) | H | \phi_A(\vec{r}) \rangle + e^{i\vec{k}\cdot\vec{a}_2} \langle \phi_B(\vec{r} - \vec{\delta}_2) | H | \phi_A(\vec{r}) \rangle + e^{i\vec{k}\cdot\vec{a}_1} \langle \phi_B(\vec{r} - \vec{\delta}_3) | H | \phi_A(\vec{r}) \rangle$$

$$S_{12} = \langle \phi_A(\vec{r}) | \phi_B(\vec{r}-\vec{\delta}_1) \rangle + e^{-i\vec{k}\cdot\vec{a}_2} \langle \phi_A(\vec{r}) | \phi_B(\vec{r}-\vec{\delta}_2) \rangle + e^{-i\vec{k}\cdot\vec{a}_1} \langle \phi_A(\vec{r}) | \phi_B(\vec{r}-\vec{\delta}_3) \rangle$$

$$S_{21} = \langle \phi_B(\vec{r}-\vec{\delta}_1) | \phi_A(\vec{r}) \rangle + e^{i\vec{k}\cdot\vec{a}_2} \langle \phi_B(\vec{r}-\vec{\delta}_2) | \phi_A(\vec{r}) \rangle + e^{i\vec{k}\cdot\vec{a}_1} \langle \phi_B(\vec{r}-\vec{\delta}_3) | \phi_A(\vec{r}) \rangle$$

$$S_{12} = s\left[1 + e^{-i\vec{k}\cdot\vec{a}_2} + e^{-i\vec{k}\cdot\vec{a}_1}\right]$$

$$S_{21} = s\left[1 + e^{i\vec{k}\cdot\vec{a}_2} + e^{i\vec{k}\cdot\vec{a}_1}\right]$$

$$H_{12} = -t\left[1 + e^{-i\vec{k}\cdot\vec{a}_2} + e^{-i\vec{k}\cdot\vec{a}_1}\right]$$

$$H_{21} = -t\left[1 + e^{i\vec{k}\cdot\vec{a}_2} + e^{i\vec{k}\cdot\vec{a}_1}\right]$$

$$t = -\langle \phi_A(\vec{r}) | H | \phi_B(\vec{r}-\vec{\delta}_1) \rangle$$

$$S = \langle \phi_A(\vec{r}) | \phi_B(\vec{r} - \vec{S}_1) \rangle$$

—— o ——

$$\det \begin{bmatrix} E_A - E_k & H_{12} - E_k S_{12} \\ H_{21} - E_k S_{21} & E_B - E_k \end{bmatrix} = 0$$

$E_A = E_B = E$

$$(E_0 - E_k)^2 - (H_{12} - E_k S_{12})(H_{21} - E_k S_{21}) = 0$$

$$E_k^2 - 2E_0 E_k - [H_{12} H_{21} + E_k^2 S_{12} S_{21}$$

$$- E_k (S_{12} H_{21} + S_{21} H_{12})] + E_0^2 = 0$$

$$E_k^2 (1 - S_{12} S_{21}) + E_k (S_{12} H_{21} + S_{21} H_{12} - 2E$$

$$+ E_0^2 - H_{12} H_{21} = 0$$

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$$E_k = \frac{1}{2(1-S_{12}S_{21})}\Big[(2E_0 - S_{12}H_{21} - S_{21}H_{12})$$

$$\mp \sqrt{(2E_0 - S_{12}H_{21} - S_{21}H_{12})^2 - 4(1-S_{12}S_{21})(E_0^2 - H_{12}}$$

— o —

$$S_{12}H_{21} = -st\left[1 + e^{-i\vec{k}\cdot\vec{a}_2} + e^{-i\vec{k}\cdot\vec{a}_1}\right]\left[1 + e^{i\vec{k}\cdot\vec{a}_2} + e^{i\vec{k}\cdot}\right.$$

$$= -st\Big[1 + 2\cos(\vec{k}\cdot\vec{a}_2) + 2\cos(\vec{k}\cdot\vec{a}_1)$$

$$+ 2 + e^{i\vec{k}\cdot(\vec{a}_1-\vec{a}_2)} + e^{-i\vec{k}\cdot(\vec{a}_1-\vec{a}_2)}\Big]$$

$$= -st\Big[3 + 2\cos(\vec{k}\cdot\vec{a}_2) + 2\cos(\vec{k}\cdot\vec{a}_1)$$

$$+ 2\cos\vec{k}\cdot(\vec{a}_1-\vec{a}_2)\Big]$$

— o —

$$S_{21}H_{12} = S_{12}H_{21}$$

$$S_{12}S_{21} = s^2\Big[3 + 2\cos(\vec{k}\cdot\vec{a}_2) + 2\cos(\vec{k}\cdot\vec{a}_1)$$

$$+ 2\cos\vec{k}\cdot(\vec{a}_1 - \vec{a}_2)\Big]$$

$$H_{12}H_{21} = t^2\Big[\quad " \quad\quad " \quad\Big]$$

SATAG

$$g(k) = 3 + 2\cos(\vec{k}\cdot\vec{a}_1) + 2\cos \vec{k}\cdot\vec{a}_2$$
$$+ 2\cos \vec{k}\cdot(\vec{a}_1 - \vec{a}_2)$$

$$S_{12} S_{21} = s^2\, g(k)$$

$$H_{12} H_{21} = t^2\, g(k)$$

$$S_{12} H_{21} = S_{21} H_{12} = -st\, g(k)$$

$$E_k = \frac{1}{\left[1 - s^2 g(k)\right]} \Big[E_0 + st\, g(k)$$

$$\mp \sqrt{\left(E_0^2 s^2 + 2E_0 st + t^2\right) g(k)} \Big]$$

$$= \frac{1}{\left[1 - s^2 g(k)\right]} \Big[E_0 + st\, g(k)$$

$$\mp \left(E_0 s + t\right) \sqrt{g(k)} \Big]$$

$$\boxed{E_k = \frac{1}{\left[1 - s^2 g(k)\right]} \left[E_0 \left(1 \mp s\sqrt{g(k)}\right) + st\, g(k) \pm t\sqrt{g(k)} \right]}$$

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$E_0 = 0$ alalım
$s \to 0$ alalım

$$\boxed{E_k = \mp t\sqrt{g(k)}}$$

$\cos(a \mp b) = \cos a \cos b \pm \sin a \sin b$

özdeşliğini kullanırsak

$$g(k) = 3 + 2\cos(k_x a_{1x} + k_y a_{1y})$$
$$+ 2\cos(k_x a_{2x} + k_y a_{2y})$$
$$+ 2\cos\left(k_x(a_{1x} - a_{2x}) + k_y(a_{1y} - a_{2y})\right)$$

$$g(k) = 3 + 2\cos\left(\frac{3}{2}k_x a + \frac{\sqrt{3}}{2}k_y a\right)$$
$$+ 2\cos\left(\frac{3}{2}k_x a - \frac{\sqrt{3}}{2}k_y a\right)$$
$$+ 2\cos\sqrt{3}k_y a$$

$$= 3 + 4\cos\frac{3}{2}k_x a \cos\frac{\sqrt{3}}{2}k_y a$$
$$+ 2\cos\sqrt{3}k_y a$$

$$E_k = \mp t\sqrt{3+4\cos\frac{3}{2}k_x a\,\cos\frac{\sqrt{3}}{2}k_y a+2\cos\sqrt{3}\,k_y}$$

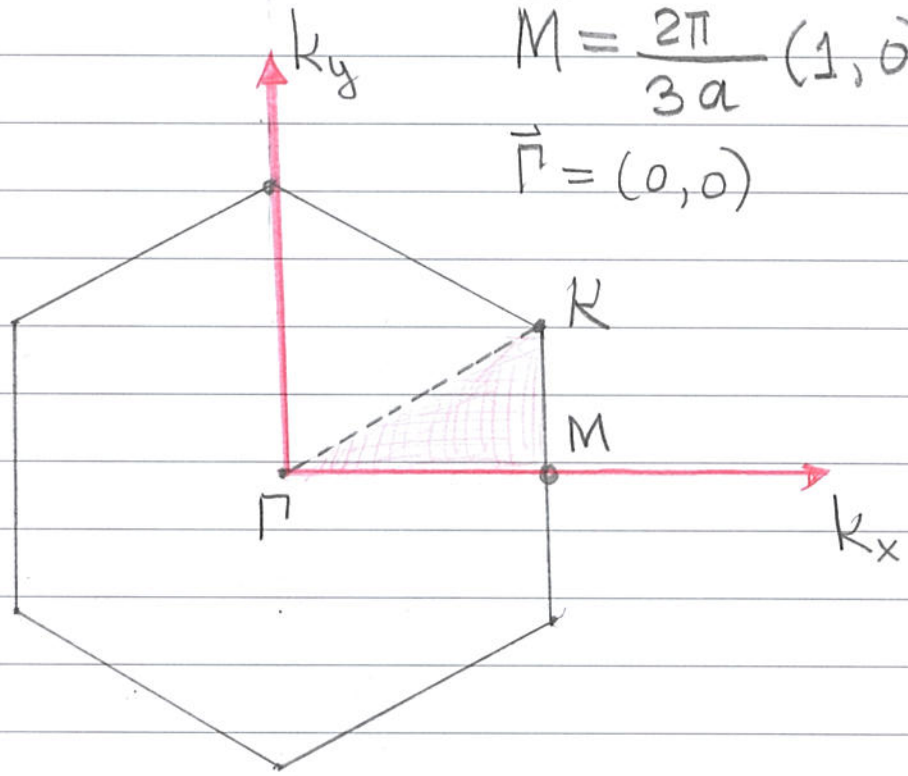
$a = 1.42$ A°

$t \cong 3$ eV

$\vec{K} = \frac{2\pi}{3a}\left(1, \frac{\sqrt{3}}{3}\right)$

$\vec{M} = \frac{2\pi}{3a}(1, 0)$

$\vec{\Gamma} = (0, 0)$



Grafen Brillouin Bölgesi

Enerji-k grafiği $\Gamma \to M \to K \to \Gamma$

doğrultuları boyunca çizilecektir.