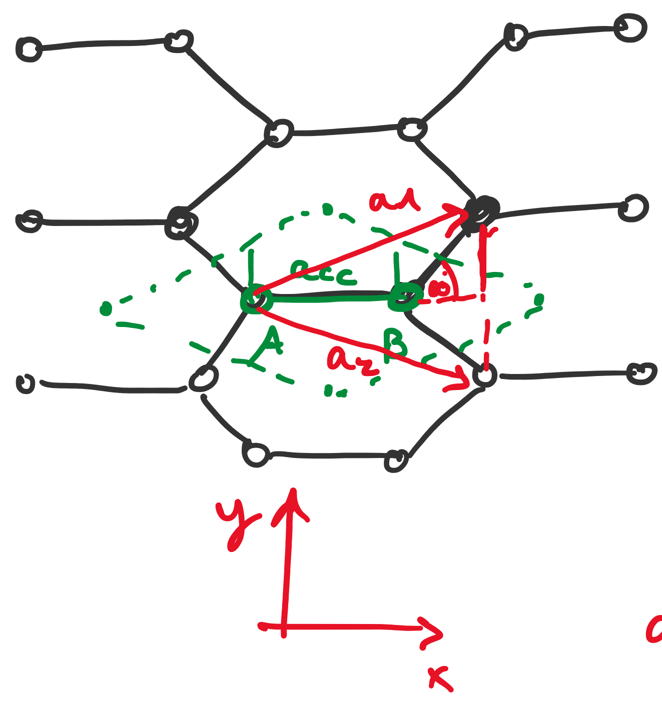
Friday, 29 November 2019 10:01

$a_{cc} = 0{,}142 \text{ nm}$



$$\underset{[2\times 2]}{H} = \begin{bmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{bmatrix}$$

singolo orbitale P_z e 1 solo primo vicino

$$H_{AB} = H_{BA}^{*}$$

$$a_1 = \begin{pmatrix} \frac{3}{2} a_{cc} \\ \frac{a_{cc}\sqrt{3}}{2} \end{pmatrix} \qquad \underline{a = \sqrt{3}\, a_{cc}}$$

$$a_2 = \begin{pmatrix} \frac{3}{2} a_{cc} \\ -\frac{a_{cc}\sqrt{3}}{2} \end{pmatrix} \qquad a_1 = \begin{pmatrix} \frac{\sqrt{3}a}{2} \\ \frac{a}{2} \end{pmatrix}$$

$$k = \begin{pmatrix} k_x \\ k_y \end{pmatrix} \qquad a_2 = \begin{pmatrix} \frac{\sqrt{3}a}{2} \\ -\frac{a}{2} \end{pmatrix}$$

$$H_{AA} = H_{BB} = \mathcal{E}_G$$

$$t = -2{,}7 \text{ eV}$$

$$H_{AB} = t + t e^{-j a_1 k} + t e^{-j a_2 k}$$

$$H_{AB} = t \underbrace{\left(1 + e^{-j a_1 \cdot k} + e^{-j a_2 \cdot k}\right)}_{f(k)} = t\left[1 + e^{-j\left(k_x \frac{\sqrt{3}a}{2} + k_y \frac{a}{2}\right)} + e^{-j\left(k_x \frac{\sqrt{3}a}{2} - k_y \frac{a}{2}\right)}\right] =$$

$$= t\left[1 + \underline{e^{-j \frac{k_x\sqrt{3}a}{2}}}\, e^{-j k_y \frac{a}{2}} + \underline{e^{-j\frac{k_x \sqrt{3}a}{2}}}\, e^{j k_y \frac{a}{2}}\right] = t\left[1 + e^{-j\frac{k_x\sqrt{3}a}{2}} \underbrace{\left(e^{-j k_y \frac{a}{2}} + e^{j k_y \frac{a}{2}}\right)}_{2\cos\left(k_y \frac{a}{2}\right)}\right] =$$

$$= t \underbrace{\left[1 + 2 e^{-j\frac{k_x \sqrt{3}a}{2}} \cos\left(k_y \frac{a}{2}\right)\right]}_{f(k)}$$

$$H = \begin{bmatrix} \mathcal{E}_G & t f(k) \\ t f^{*}(k) & \mathcal{E}_G \end{bmatrix} \qquad \det\left(EI - H\right) = 0$$

$$\left(E - \mathcal{E}_G\right)^2 - t^2 \left|f(k)\right|^2 = 0$$

$$E^2 - 2\mathcal{E}_G E + \mathcal{E}_G^2 - t^2 \left|f(k)\right|^2 = 0$$

$$E(k) = \mathcal{E}_G \pm t\sqrt{\left|f(k)\right|^2}$$

$$\left|f(k)\right|^2 = f(k)\cdot f(k)^{*} = \left[1 + 2e^{-j\frac{k_x\sqrt{3}a}{2}} \cos\left(k_y\frac{a}{2}\right)\right]\left[1 + 2e^{j\frac{k_x\sqrt{3}a}{2}}\cos\left(k_y \frac{a}{2}\right)\right] =$$

$$= 1 + 2e^{j\frac{k_x\sqrt{3}a}{2}}\cos\left(k_y\frac{a}{2}\right) + 2e^{-j\frac{k_x\sqrt{3}a}{2}}\cos\left(k_y \frac{a}{2}\right) + 4\cos^2\left(k_y\frac{a}{2}\right) =$$

$$= 1 + 2\cos\left(k_y\frac{a}{2}\right) \underbrace{\left[e^{j\frac{k_x\sqrt{3}a}{2}} + e^{-j\frac{k_x\sqrt{3}a}{2}}\right]} + 4\cos^2\left(k_y \frac{a}{2}\right) =$$

$$= 1 + 4\cos\left(k_y\frac{a}{2}\right)\cos\left(\frac{k_x\sqrt{3}a}{2}\right) + 4\cos^2\left(k_y \frac{a}{2}\right)$$

$$E(k) = \mathcal{E}_G \pm t\sqrt{\left|f(k)\right|^2} = \mathcal{E}_G \pm \sqrt{1 + 4\cos\left(k_y\frac{a}{2}\right)\cos\left(\frac{k_x\sqrt{3}a}{2}\right) + 4\cos^2\left(k_y\frac{a}{2}\right)}$$