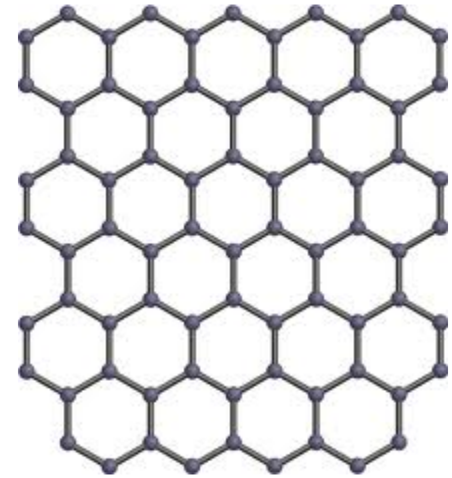
Graphene

n.b. Prof. Andrea Young new faculty!

- Single layers of honeycomb lattice of carbon
- First systematically exfoliated and studied by A. Geim + K. Novoselov, 2004.
- Nobel prize, 2011
- Interesting because it intrinsically has a *point Fermi surface*

Graphene



- electronic properties?
- Carbon has Z=6, (He) $2s^2\,2p^2$ = (He) $sp^2\pi$
- 1 $\pi = p^z$ electron per C atom not tied up in covalent sp^2 bonds
- Can treat this via tight-binding model

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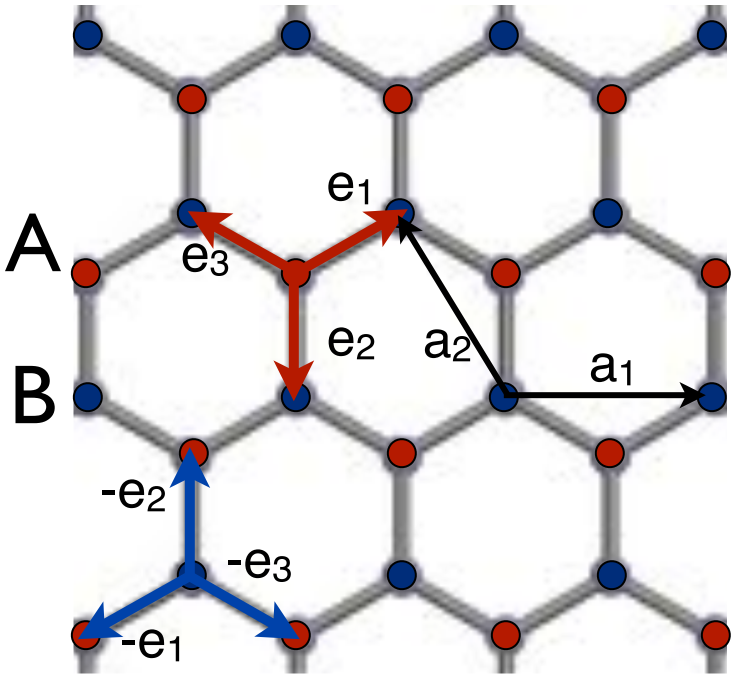
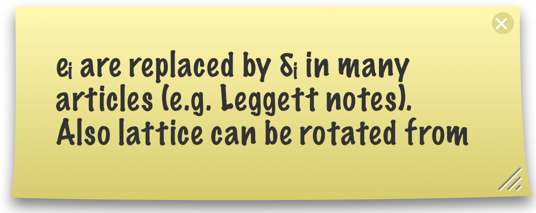


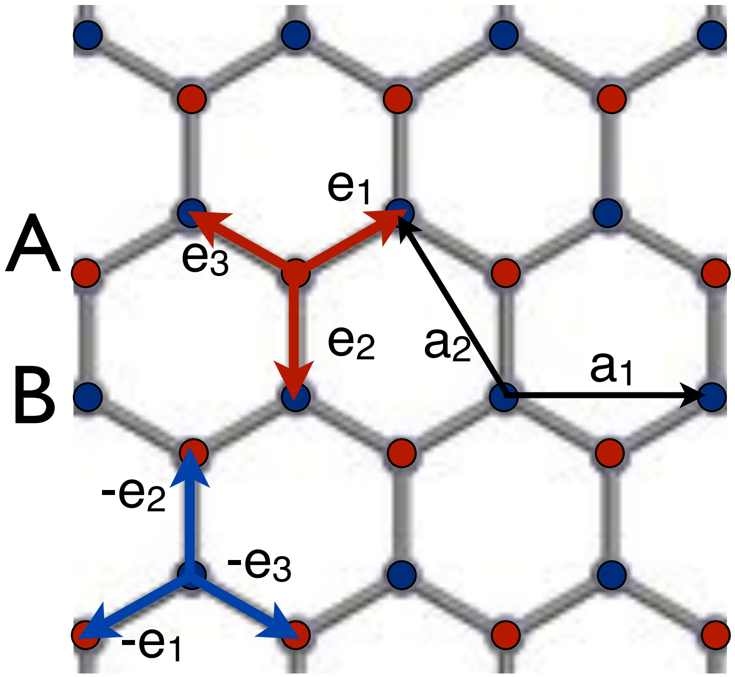


Bipartite: A sites hop to B sites, and vice versa

$$\hat{H}\psi_R = \epsilon_0\psi_R - \gamma\sum_{i=1}^{3}\psi_{R+e_i} = \epsilon\psi_R \qquad R \in A$$

$$\hat{H}\psi_R = \epsilon_0\psi_R - \gamma\sum_{i=1}^{3}\psi_{R-e_i} = \epsilon\psi_R \qquad R \in B$$

Graphene



Bloch form:

$$\psi_R = \begin{cases} \psi_A e^{ik\cdot R} & R \in A \\ \psi_B e^{ik\cdot R} & R \in B \end{cases}$$

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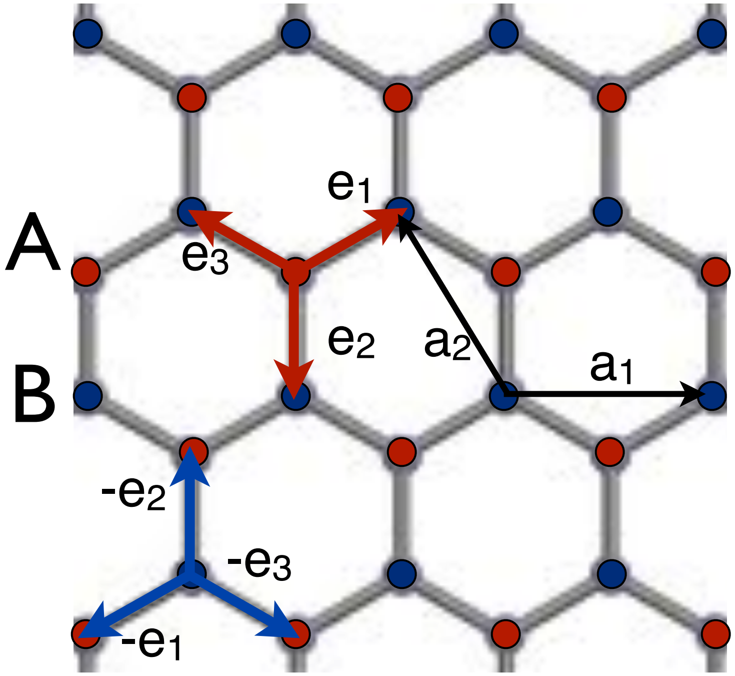

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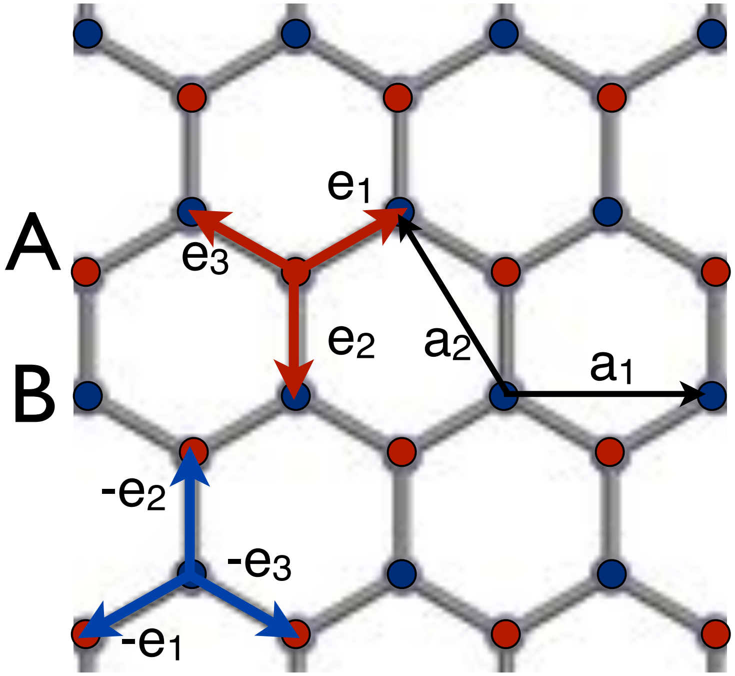
$$\begin{pmatrix} \epsilon_0 & f(k) \\ f^*(k) & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \epsilon \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

$$f(k) = -\gamma \sum_{i=1}^{3} e^{ik\cdot e_i}$$

Graphene



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energy bands

$$\epsilon_{\pm}(k) = \epsilon_0 \pm |f(k)|$$

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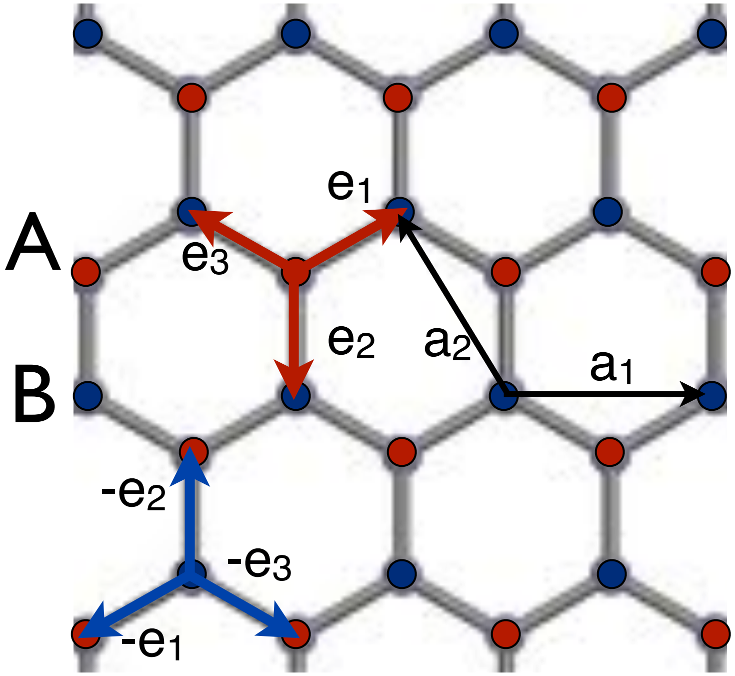

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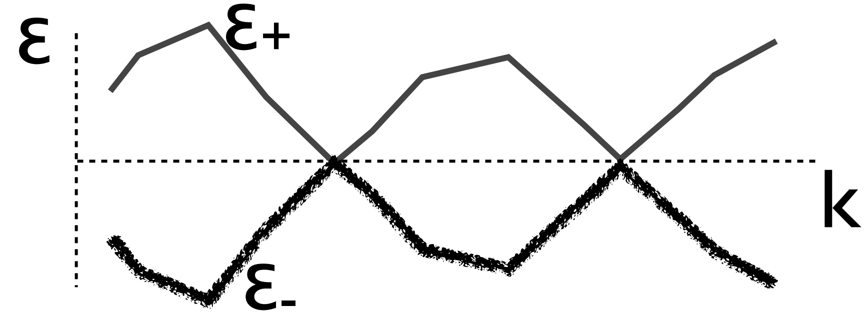
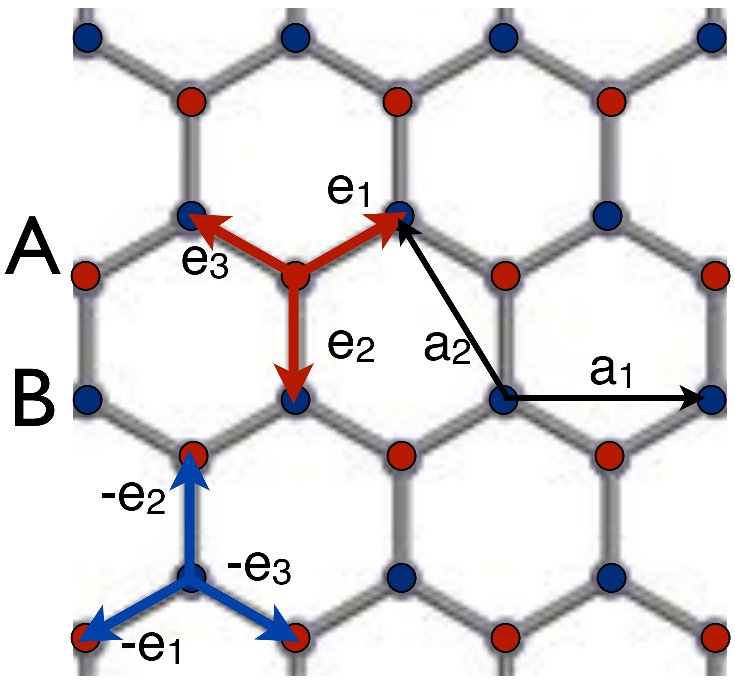


conduction and valence
band touch if and only if f=0

Graphene



$$e_1 = a_0(\frac{\sqrt{3}}{2}, \frac{1}{2})$$

$$e_2 = a_0(0, -1)$$

$$e_3 = a_0(-\frac{\sqrt{3}}{2}, \frac{1}{2}) = -e_1 - e_2$$

$$f(k) = -\gamma \left[e^{-ik_y a_0} + 2\cos\left(\frac{\sqrt{3}k_x a_0}{2}\right) e^{ik_y a_0/2} \right]$$

$$= -\gamma e^{\frac{i}{2}k_y a_0} \left[e^{-\frac{3}{2}ik_y a_0} + 2\cos\left(\frac{\sqrt{3}k_x a_0}{2}\right) \right]$$

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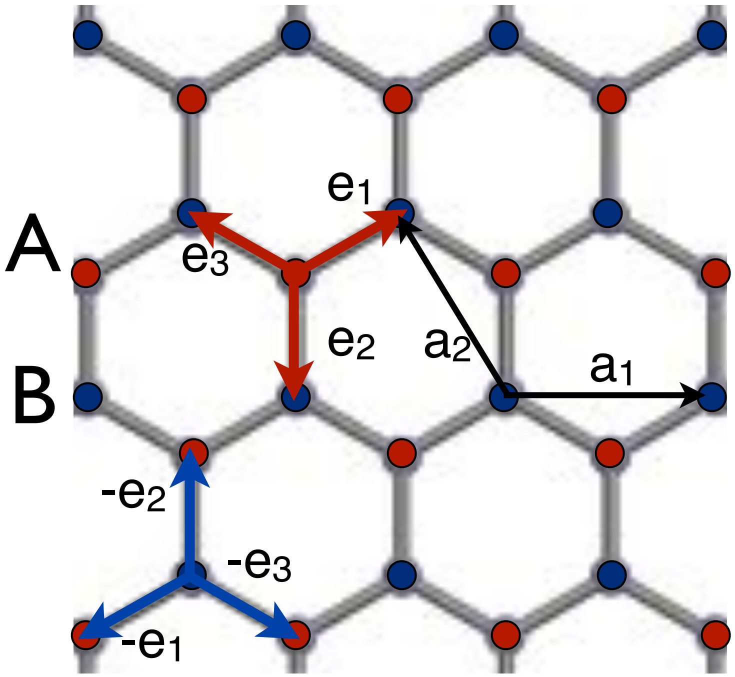

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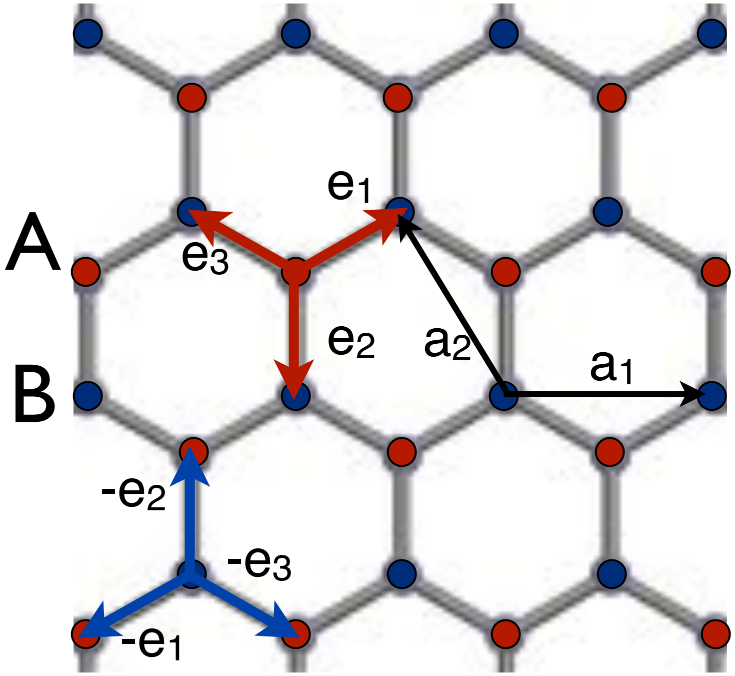
$$e_2 = a_0(0, -1)$$
$$e_3 = a_0\left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right) = -e_1 - e_2$$

$$\sin\left(\tfrac{3}{2}k_y a_0\right) = 0 \quad \Rightarrow \quad k_y = 0, \pm\frac{2\pi}{3a_0}, \cdots$$

$$\cos\left(\tfrac{3}{2}k_y a_0\right) + 2\cos\left(\frac{\sqrt{3}}{2}k_x a_0\right) = 0$$

Graphene



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$$\sin\left(\tfrac{3}{2}k_y a_0\right) = 0 \quad \Longrightarrow \quad k_y = 0, \pm\frac{2\pi}{3a_0}, \cdots$$

$$\pm 1 + 2\cos\left(\frac{\sqrt{3}}{2}k_x a_0\right) = 0 \qquad k_x = \pm\frac{4\pi}{3\sqrt{3}a_0}, \pm\frac{2\pi}{3\sqrt{3}a_0}, \cdots$$

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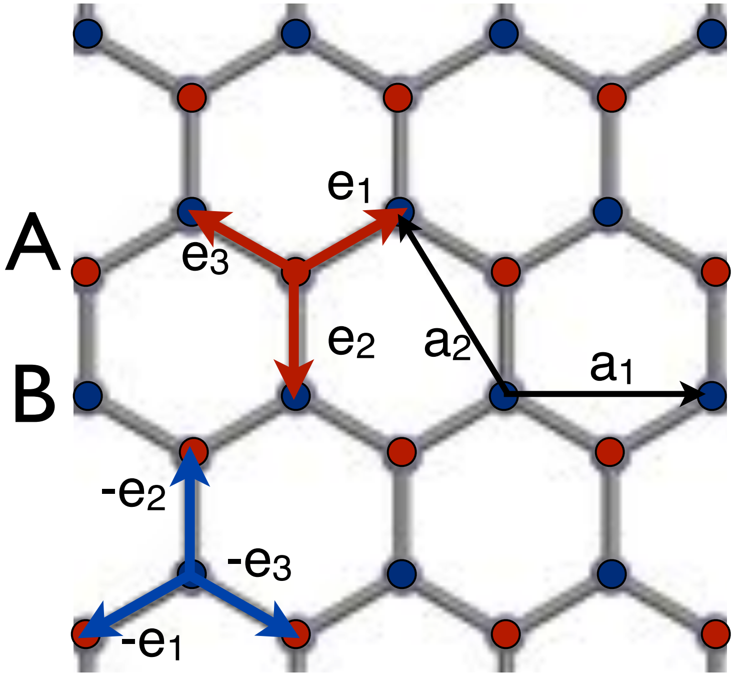

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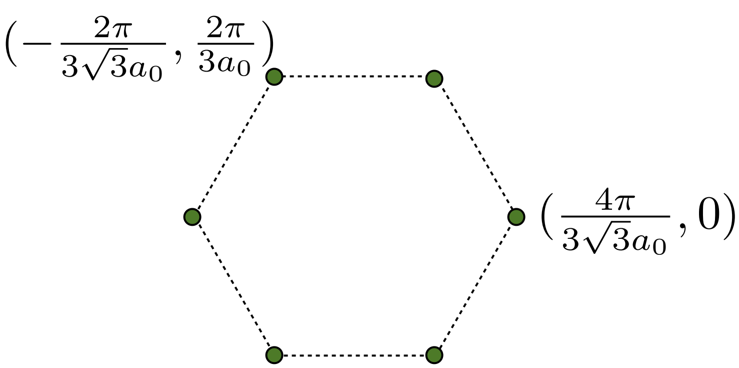

$$k_y = 0, \pm\frac{2\pi}{3a_0}, \cdots$$

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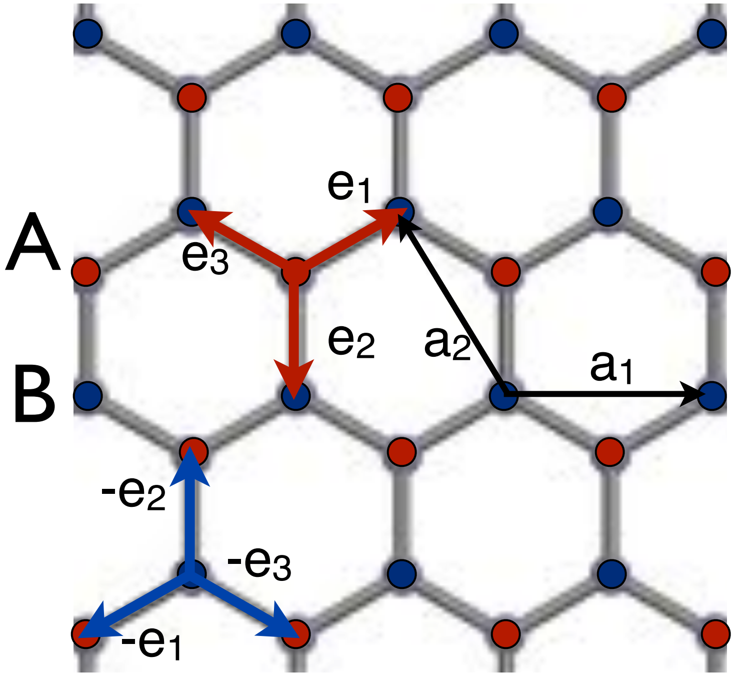

$$e_1 = a_0\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$$

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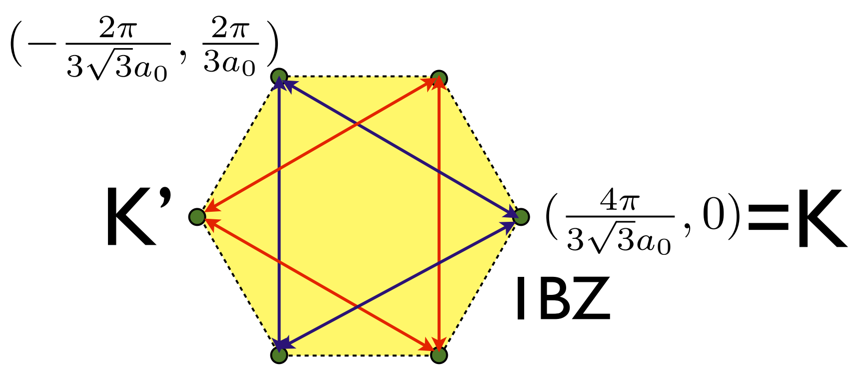
$$a_1 = e_1 - e_3 = \sqrt{3}a_0(1, 0)$$

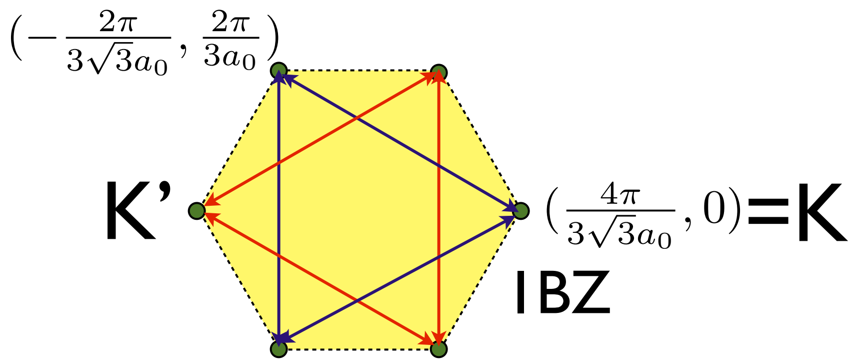
$$a_2 = e_3 - e_2 = \sqrt{3}a_0\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$$



$$b_1 = \left(\frac{2\pi}{\sqrt{3}a_0}, \frac{2\pi}{3a_0}\right)$$

$$b_2 = \left(0, \frac{4\pi}{3a_0}\right)$$

Graphene



- Result: *zero gap* semiconductor with *Fermi points*
- Low energy excitations?

$$f(K+q) \approx \frac{3}{2}\gamma a_0(q_x + iq_y) \qquad f(K'+q) \approx -\frac{3}{2}\gamma a_0(q_x - iq_y)$$

$$\epsilon_\pm(K(K')+q) \approx \pm v|q| \qquad v = \frac{3}{2}\gamma a_0$$

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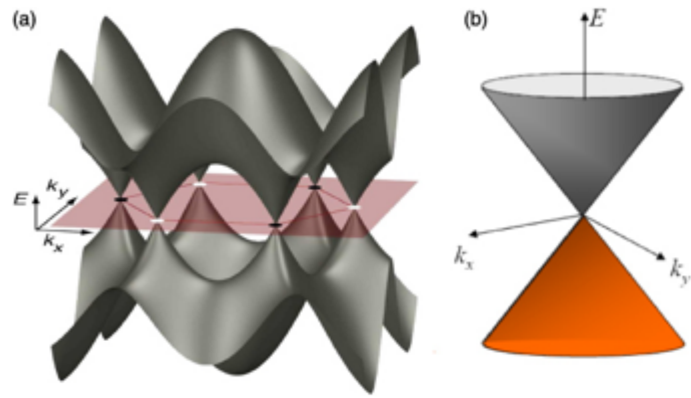

"Dirac" cones

- Result: *zero gap* semiconductor with *Fermi points*

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Dirac equation

$$\left(\begin{array}{cc} \epsilon_0 & f(k) \\ f^*(k) & \epsilon_0 \end{array} \right) \left(\begin{array}{c} \psi_A \\ \psi_B \end{array} \right) = \epsilon \left(\begin{array}{c} \psi_A \\ \psi_B \end{array} \right)$$

Expand near K point: $f(K+q) \approx \frac{3}{2}\gamma a_0 (q_x + i q_y)$

$$\left[\epsilon_0 + v\left(q_x \underline{\sigma}^x - q_y \underline{\sigma}^y\right)\right]\psi = \epsilon\psi$$

$$\left[\epsilon_0 + v\left(q_x \gamma^x + q_y \gamma^y\right)\right]\psi = \epsilon\psi$$ 2d Dirac equation

$\gamma^x = \sigma^x \quad \gamma^y = \sigma^y$

for K point

$\gamma^x = -\sigma^x \quad \gamma^y = \sigma^y$

for K' point

Many interesting properties follow from the Dirac form