

# The ABC of graphene trilayers

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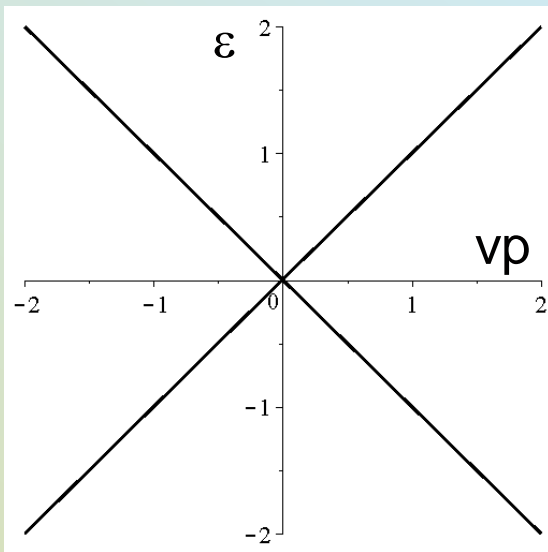
in collaboration with

Mikito Koshino

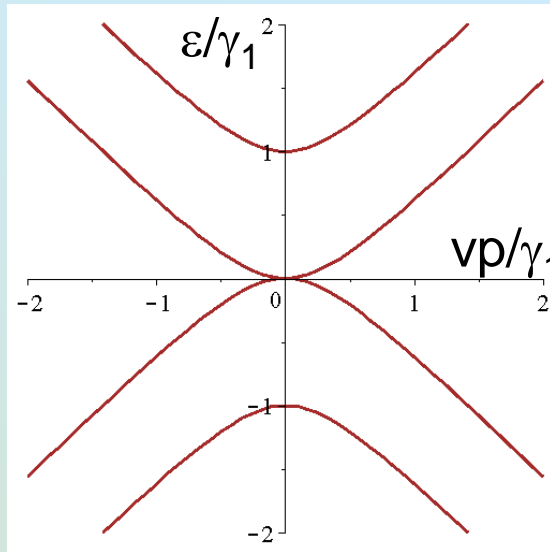
Tokyo Institute of Technology, Japan



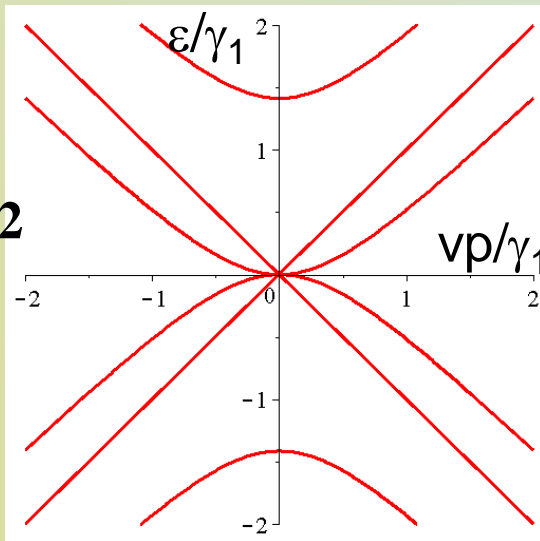
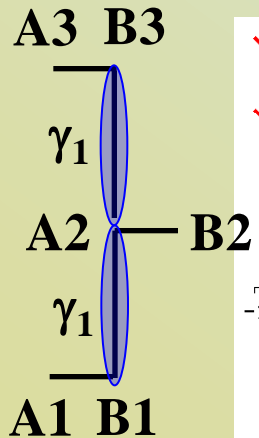
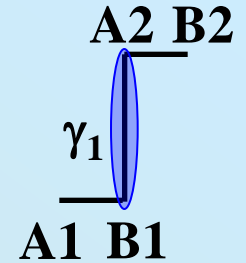
$\overline{\gamma_0}$   
A1 B1



monolayer graphene:  
Berry phase  $\pi$



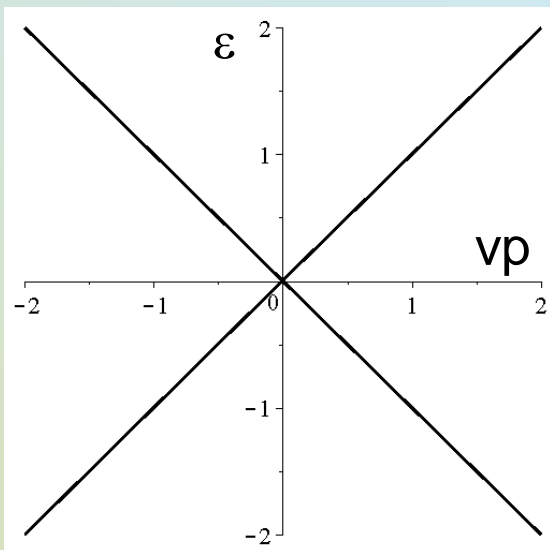
AB-stacked bilayer:  
Berry phase  $2\pi$



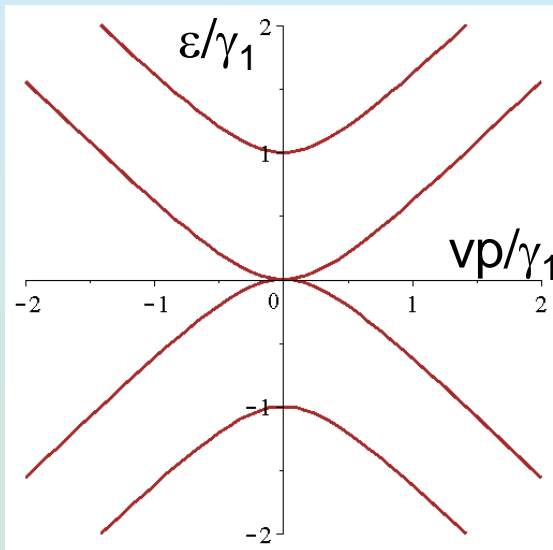
ABA-stacked trilayer:  
Berry phase  $\pi$  and  $2\pi$

a combination of  
monolayer-like and  
bilayer-like bands

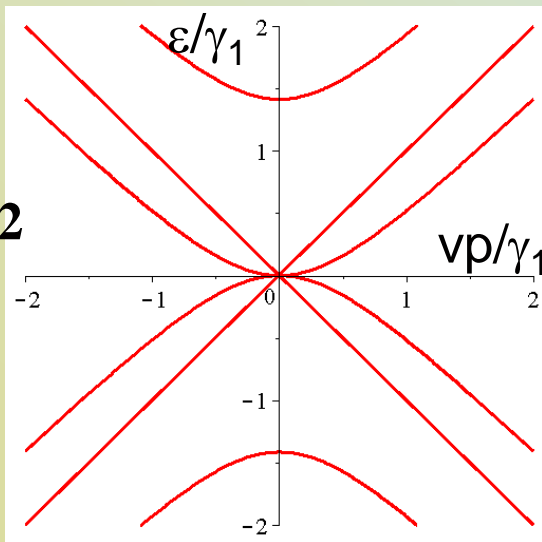
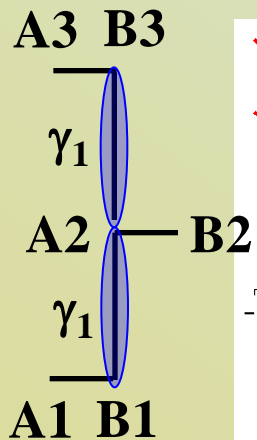
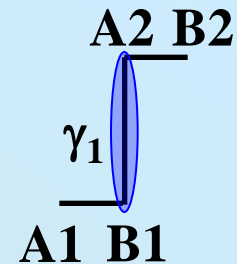
$\overline{\gamma_0}$   
A1 B1



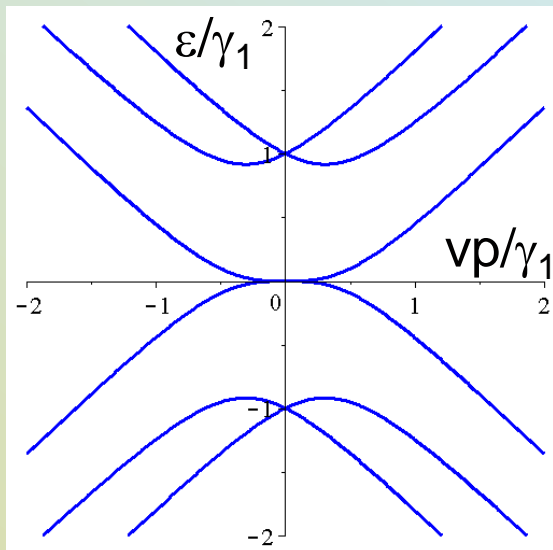
monolayer graphene:  
Berry phase  $\pi$



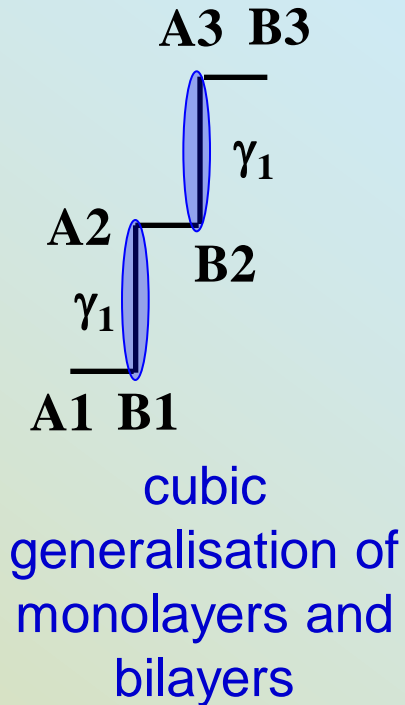
AB-stacked bilayer:  
Berry phase  $2\pi$



ABA-stacked trilayer:  
Berry phase  $\pi$  and  $2\pi$



ABC-stacked trilayer:  
Berry phase  $3\pi$



# The ABC of graphene trilayers:

using a simple (tight-binding) model,  
can we identify any novel features  
in their low-energy electronic spectrum?

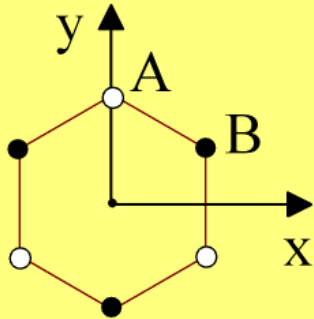
## Overview

- Review of tight-binding model of monolayers and bilayers
- ABA-stacked trilayers
- ABC-stacked trilayers

# Electronic dispersion of a monolayer

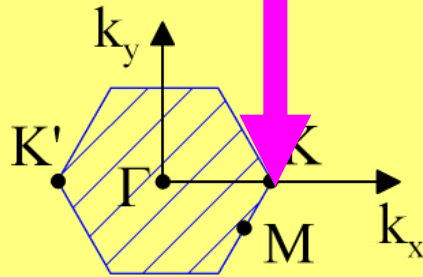
Saito *et al*, "Physical Properties of Carbon Nanotubes"  
(Imperial College Press, London, 1998)

Symmetrical  
unit cell

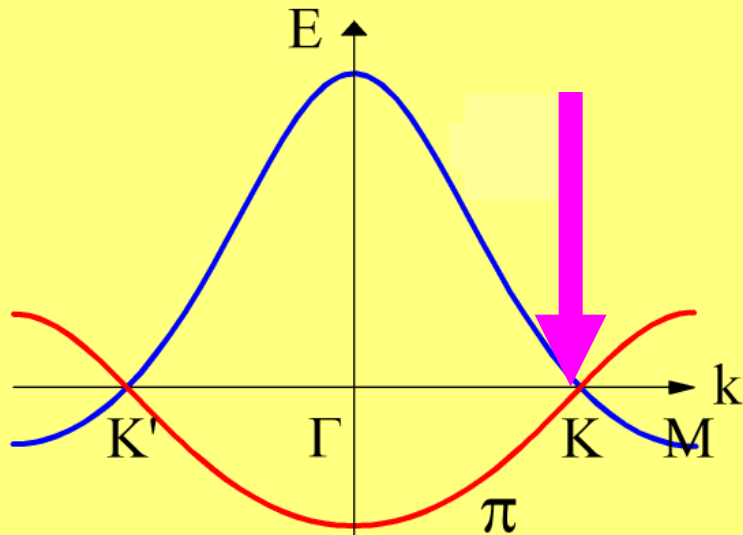


Two non-equivalent  
carbon positions

Brillouin  
zone



Two non-equivalent  
K-points

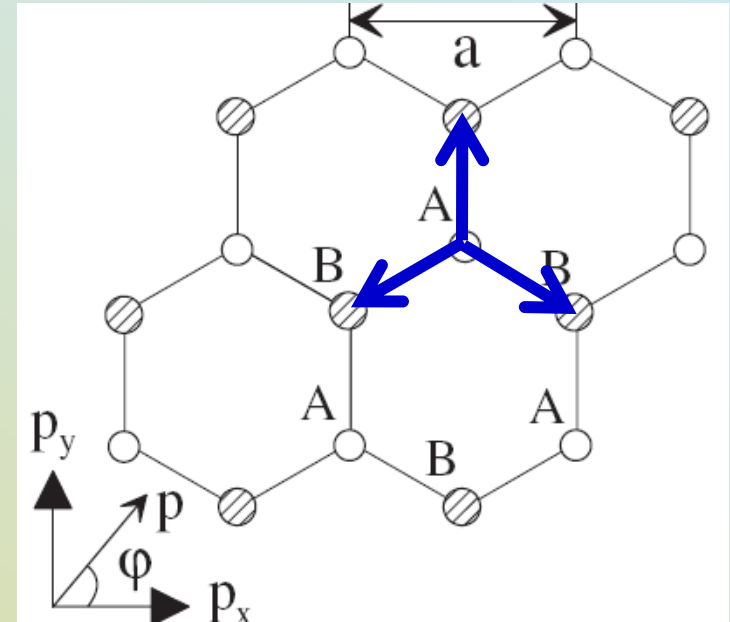


Two bands: no energy gap at the K-points

To calculate the transfer  
integral for hopping from  
site A to site B we need to  
determine factors like

$$e^{i\vec{k} \cdot (\vec{R}_B - \vec{R}_A)}$$

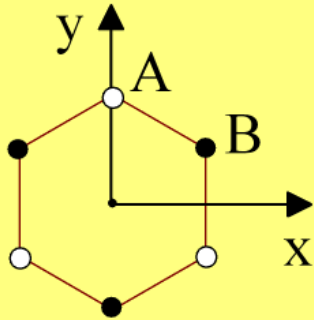
that depend on the atomic  
positions  $\vec{R}_A, \vec{R}_B$



# Electronic dispersion of a monolayer

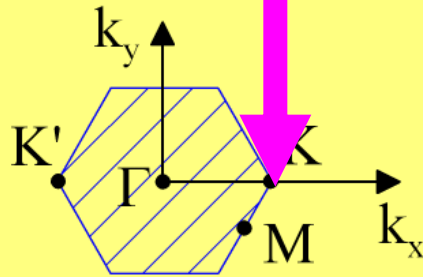
Saito *et al*, "Physical Properties of Carbon Nanotubes"  
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Symmetrical  
unit cell

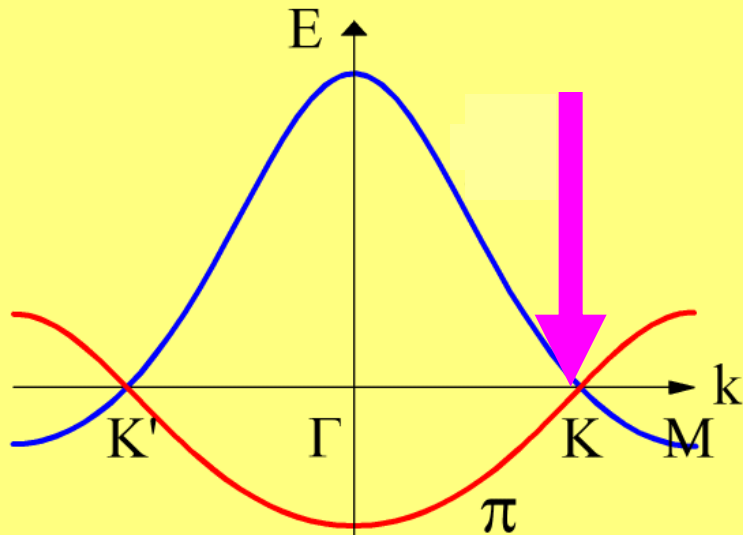


Two non-equivalent  
carbon positions

Brillouin  
zone



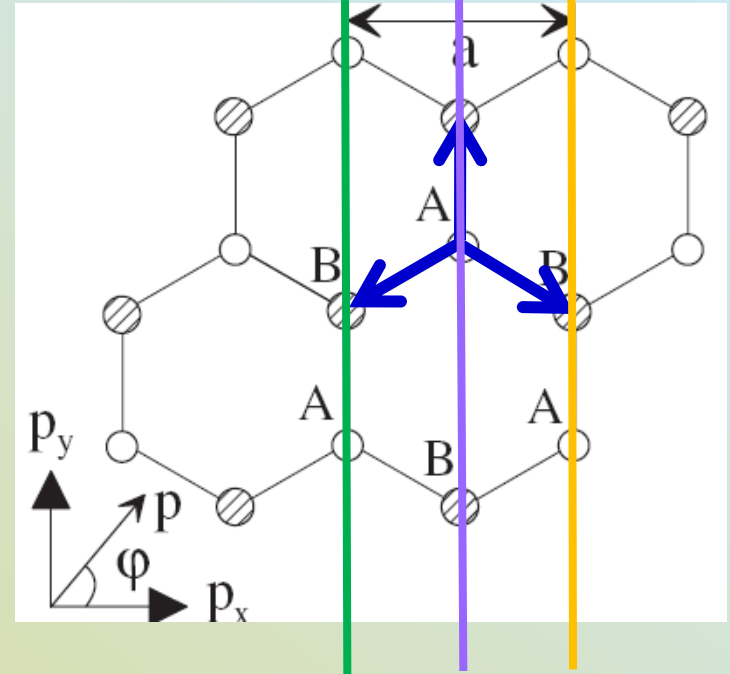
Two non-equivalent  
K-points



Two bands: no energy gap at the K-points

Exactly at the K point:  $\vec{k} = \left( \frac{4\pi}{3a}, 0 \right)$

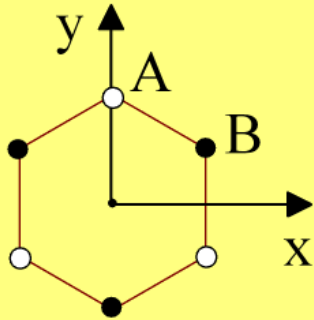
$$e^{i\vec{k} \cdot \vec{R}_i} = e^{-2\pi i/3} \quad e^{i0} \quad e^{+2\pi i/3}$$



# Electronic dispersion of a monolayer

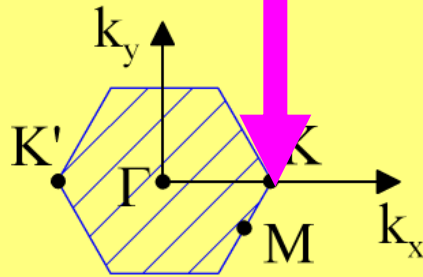
Saito *et al*, "Physical Properties of Carbon Nanotubes"  
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Symmetrical  
unit cell

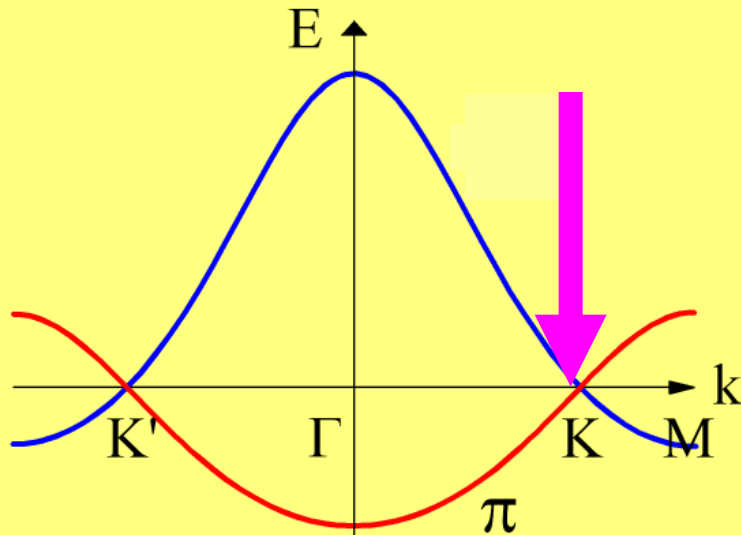


Two non-equivalent  
carbon positions

Brillouin  
zone



Two non-equivalent  
K-points

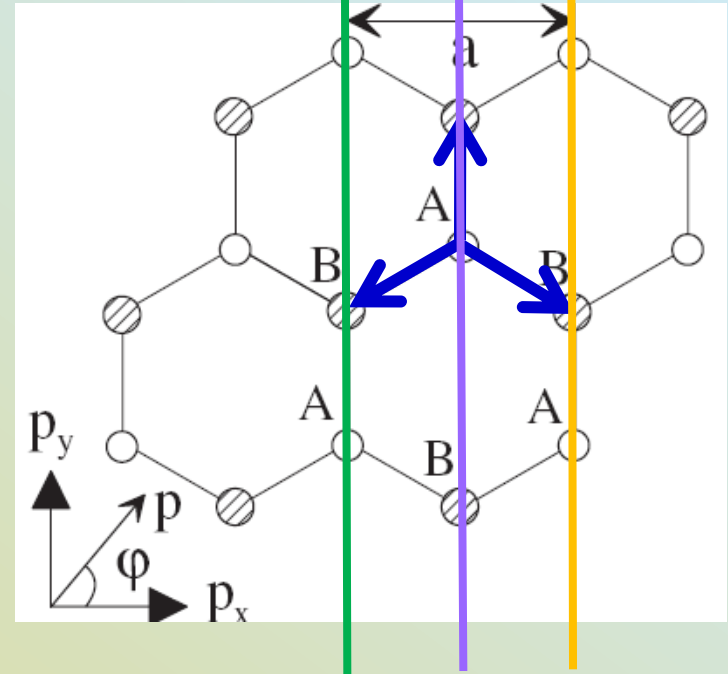


Two bands: no energy gap at the K-points

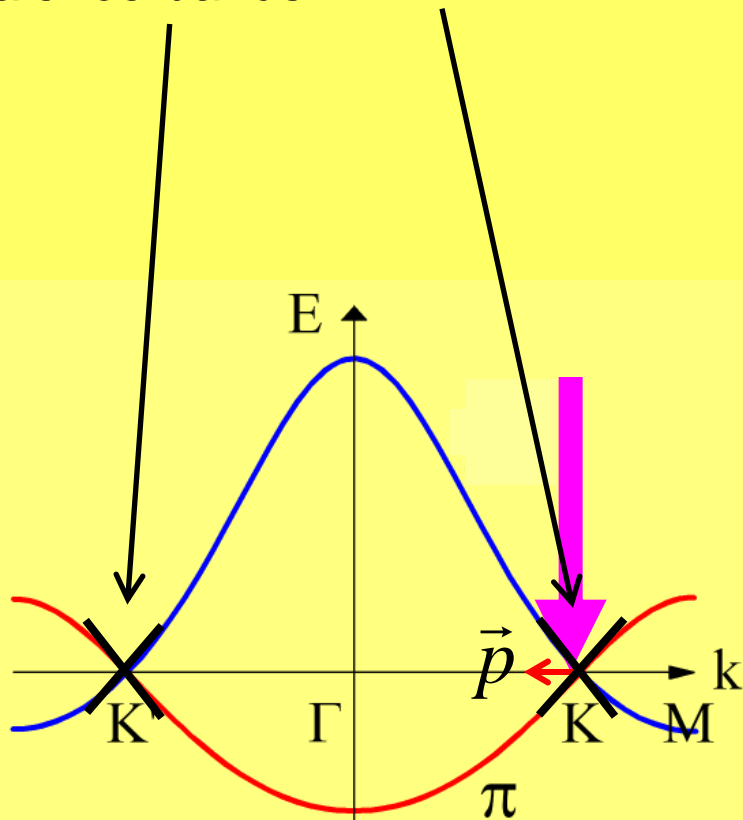
Exactly at the K point:  $\vec{k} = \left( \frac{4\pi}{3a}, 0 \right)$

Two uncoupled triangular  
sub-lattices

$$e^{-2\pi i/3} + e^{i0} + e^{+2\pi i/3} = 0$$



The Dirac Hamiltonian gives a linear spectrum  $E = v|p|$  around each K point – with no gap between conduction and valence bands.



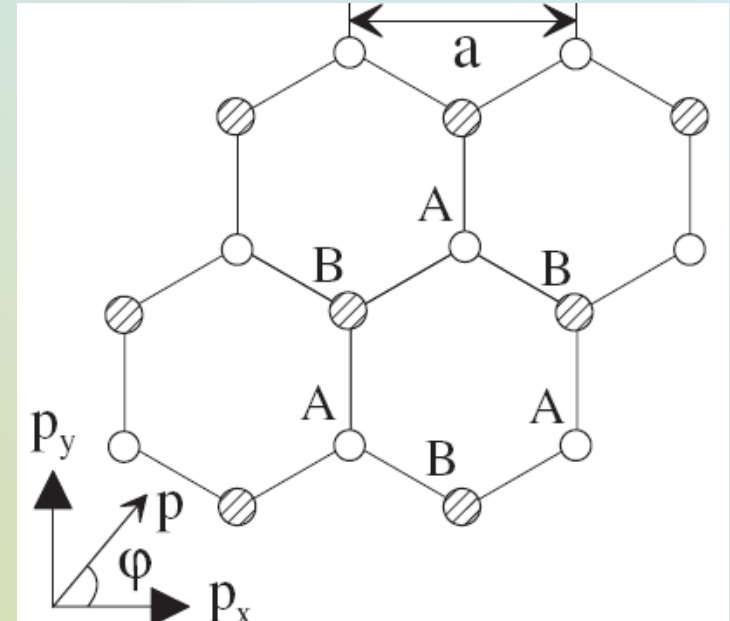
Two bands: no energy gap at the K-points

Near the K point:  $\vec{k} = \left( \frac{4\pi}{3a}, 0 \right) + \frac{\vec{p}}{\hbar}$

**Coupling between triangular sub-lattices occurs in linear-in-momentum terms:**

$$\hat{H}_1 = v \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}$$

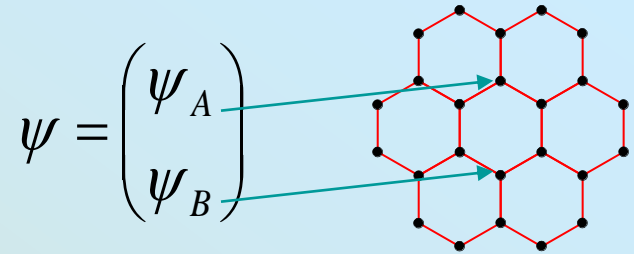
**written in a two-component basis of A and B sites.**





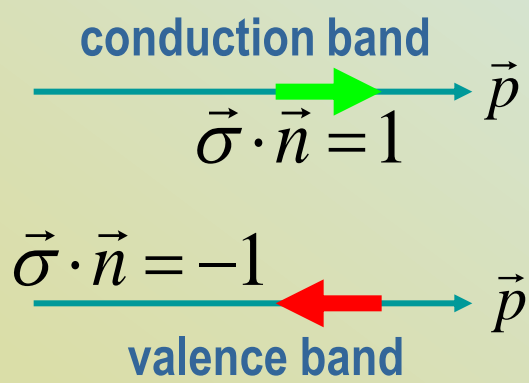
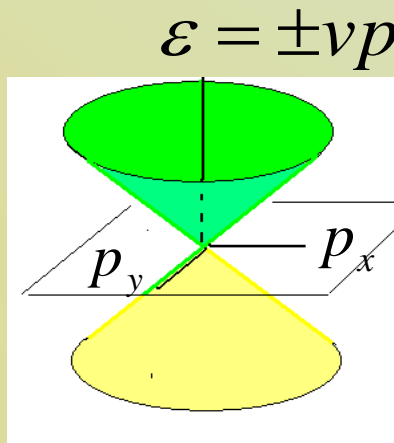
Bloch function amplitudes (e.g., in the valley K) on the AB sites ('pseudospin') mimic spin components of a relativistic particle.

Pseudospin and chirality:  
Berry's phase  $\pi$



$$\hat{H}_1 = v \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = v \vec{\sigma} \cdot \vec{p} = vp \vec{\sigma} \cdot \vec{n}$$

Chiral Dirac-type (relativistic) electrons: pseudospin of plane waves is linked to the momentum direction, which determines unusual transport properties of graphene.

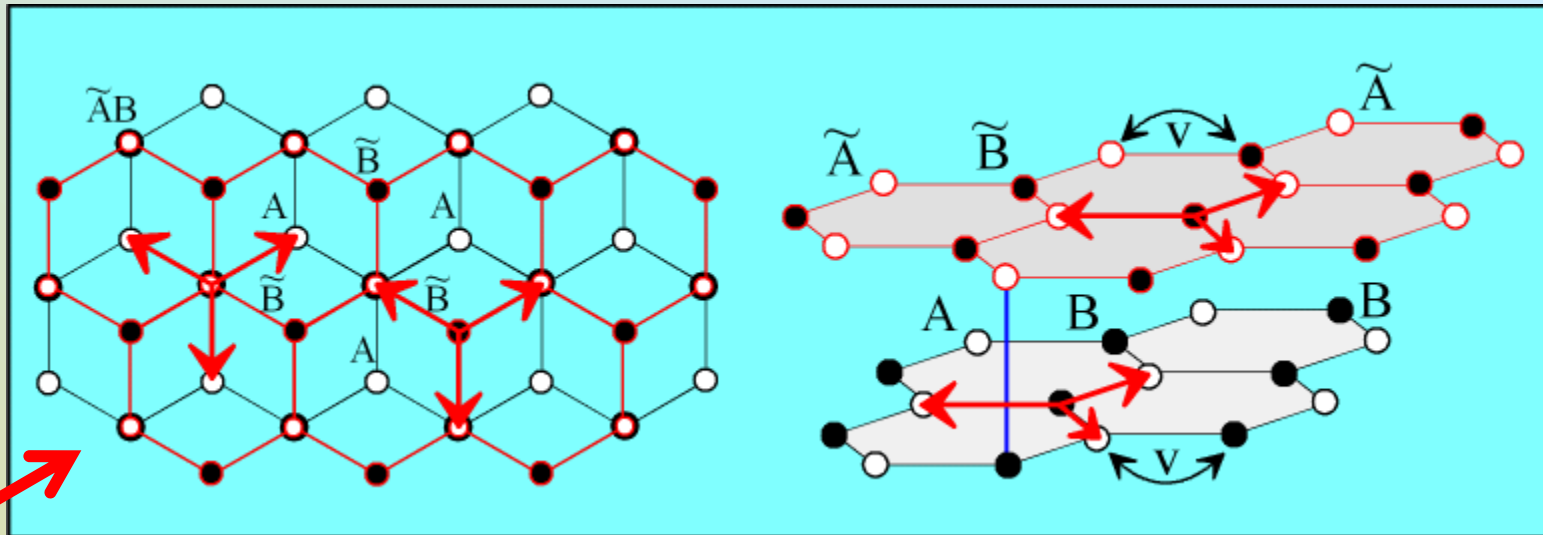


$$\vec{p} = (p \cos \varphi, p \sin \varphi)$$

$$\psi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\varphi/2} \\ \pm e^{-i\varphi/2} \end{pmatrix}$$

chiral plane wave states

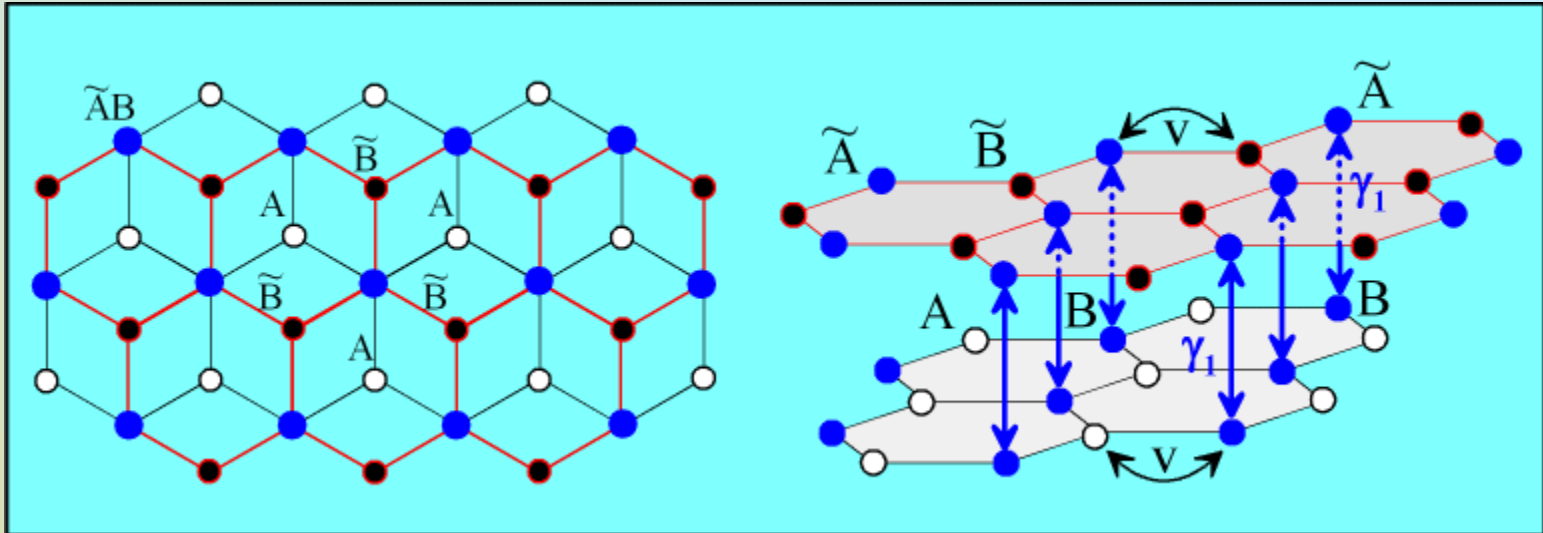
# Bilayer [Bernal (AB) stacking]



(B to A) and ( $\tilde{B}$  to  $\tilde{A}$ )  
hopping  
given by  
 $\pi^+ = p_x - ip_y$

$$H = \begin{pmatrix} A & \tilde{B} & \tilde{A} & B \\ & & v\pi & v\pi^+ \\ & v\pi^+ & & \\ v\pi & & & \end{pmatrix} \begin{pmatrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{pmatrix}$$

# Bilayer [Bernal (AB) stacking]



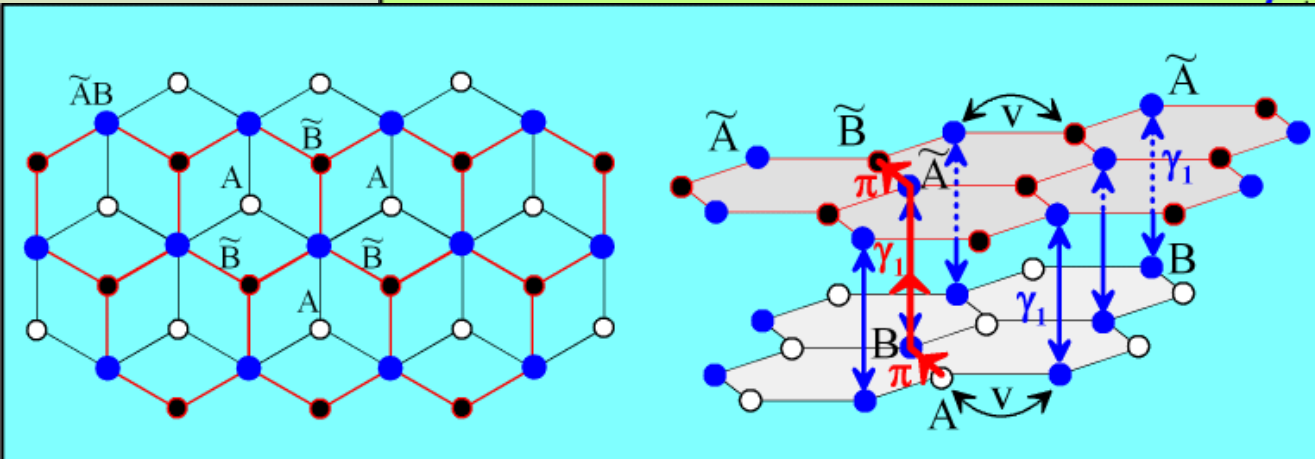
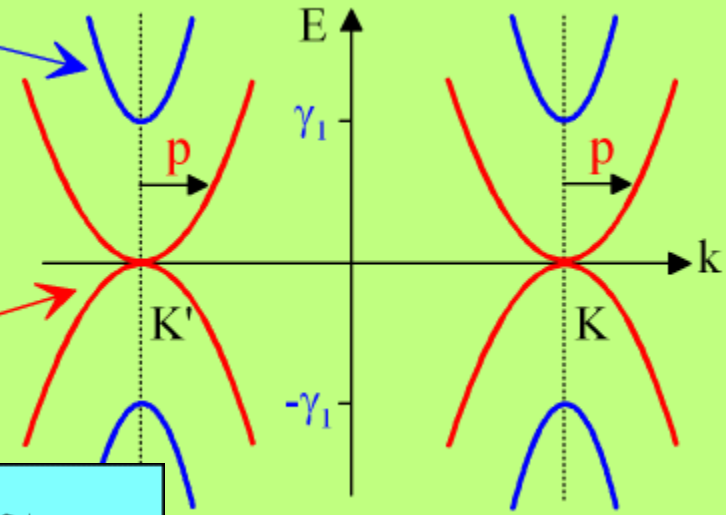
Bilayer Hamiltonian

$$H = \begin{pmatrix} A & \tilde{B} & \tilde{A} & B \\ 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^+ & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} \begin{pmatrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{pmatrix}$$

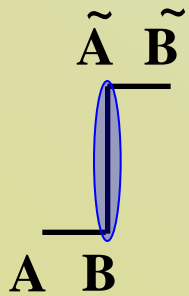
$\tilde{A}B$  orbitals form dimers  
with energy  $|E| \geq \gamma_1$

Quadratic dispersion at low energy:

$$E = \pm \frac{p^2}{2m}$$



E. McCann and V.I. Fal'ko  
PRL 96, 086805 (2006)



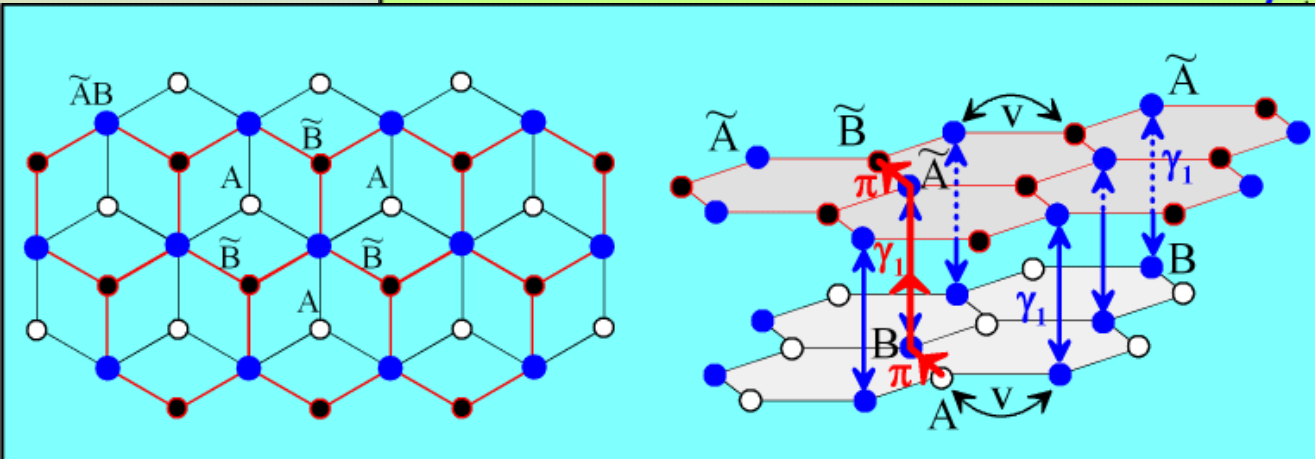
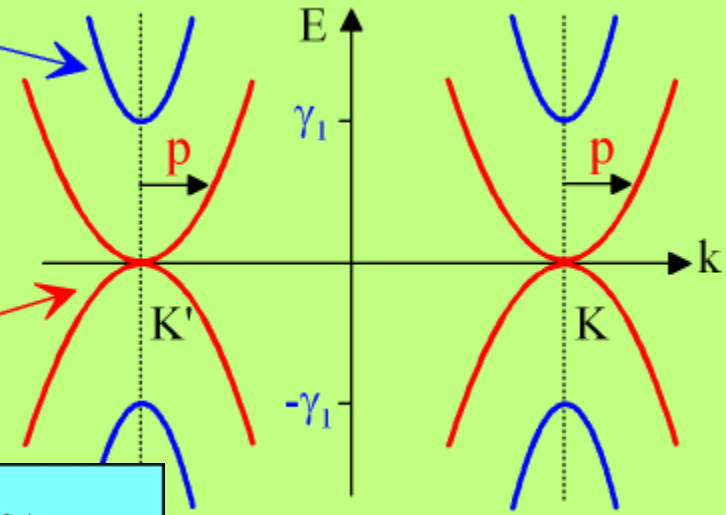
Bilayer  
Hamiltonian

$$H = \begin{pmatrix} A & \tilde{B} & \tilde{A} & B \\ 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & v\pi & 0 \\ 0 & v\pi^+ & 0 & \gamma_1 \\ v\pi & 0 & \gamma_1 & 0 \end{pmatrix} \begin{pmatrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{pmatrix}$$

$\tilde{A}\tilde{B}$  orbitals form dimers  
with energy  $|E| \geq \gamma_1$

Quadratic dispersion at low energy:

$$E = \pm \frac{p^2}{2m}$$



E. McCann and V.I. Fal'ko  
PRL 96, 086805 (2006)

Bilayer Hamiltonian written in a 2 component basis of A and  $\tilde{B}$  sites

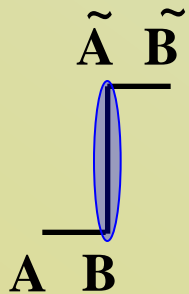
$$H = \frac{-1}{2m} \begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix}$$

mass  
 $m = \gamma_1 / v^2$

A to  $\tilde{B}$  hopping

- bottom layer A  $\rightarrow$  B (factor  $\pi$ )
- switch layers via dimer  $B\tilde{A}$  ( $\gamma_1^{-1}$ )
- top layer  $\tilde{A} \rightarrow \tilde{B}$  (factor  $\pi$ )

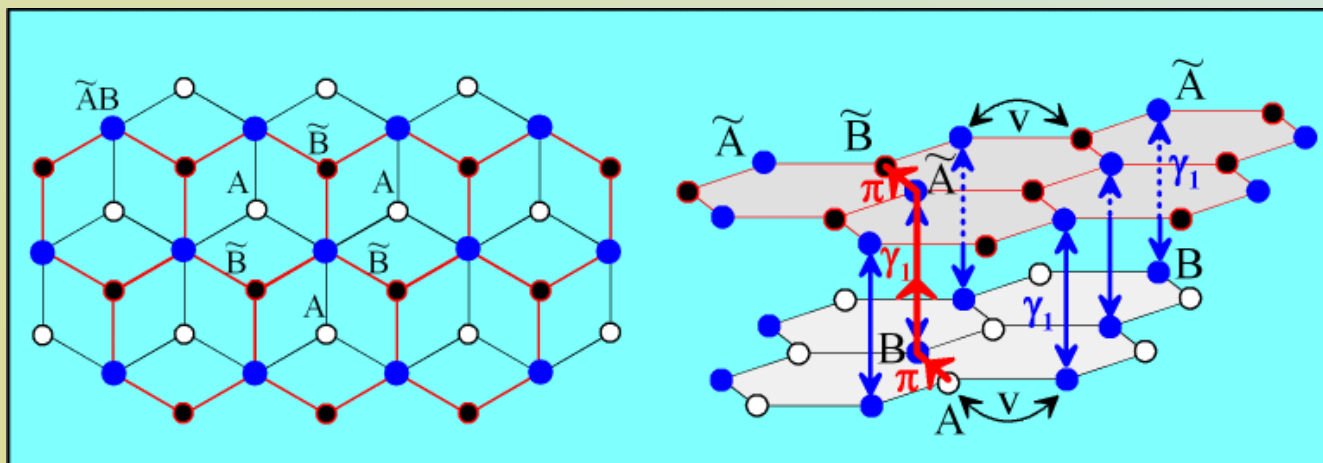
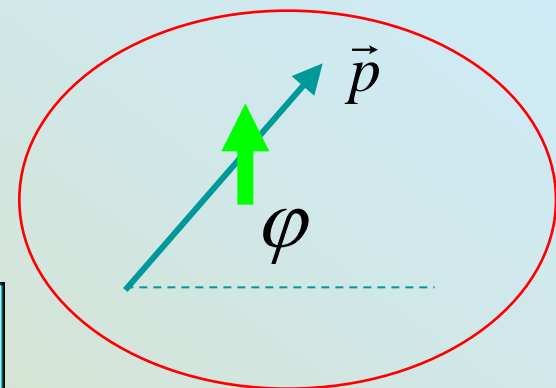
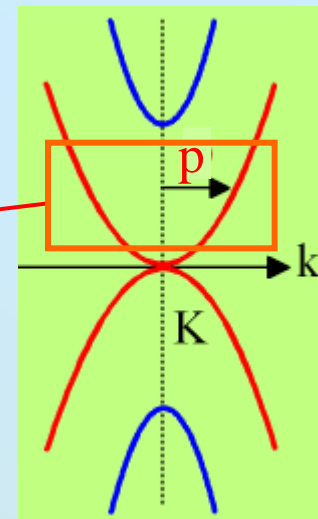
$$\pi = p_x + ip_y$$



# Chiral electrons in bilayer graphene: Berry's phase $2\pi$

$$H \approx -\frac{1}{2m} \begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} = -\frac{p^2}{2m} \begin{pmatrix} 0 & e^{-2i\varphi} \\ e^{2i\varphi} & 0 \end{pmatrix}$$

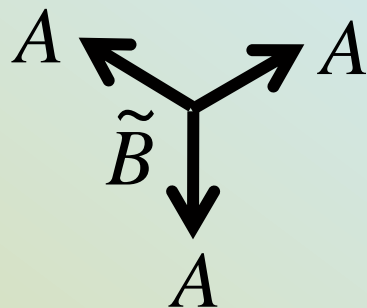
$$\varepsilon \approx \pm \frac{p^2}{2m} \iff \psi_{\pm} = \begin{pmatrix} \psi_A \\ \psi_{\tilde{B}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\varphi} \\ -e^{i\varphi} \end{pmatrix}$$



E. McCann and V.I. Fal'ko,  
PRL 96, 086805 (2006)

# Trigonal warping in bilayer graphene

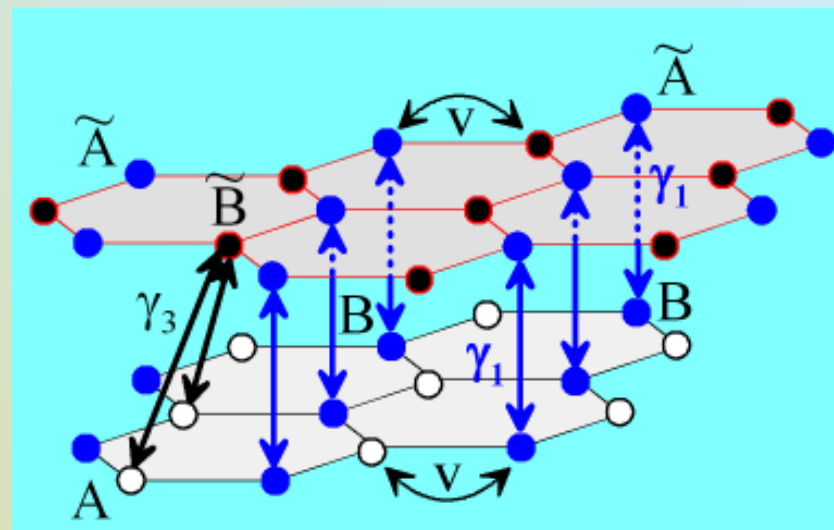
EM and V.I. Fal'ko, PRL **96**, 086805 (2006)



$$v_3 = \frac{\sqrt{3}}{2} a \gamma_3 / \hbar$$

$$\pi = p_x + ip_y$$

$$H = \begin{pmatrix} A & \tilde{B} & \tilde{A} & B \\ 0 & v_3 \pi & 0 & v \pi^+ \\ v_3 \pi^+ & 0 & v \pi & 0 \\ 0 & v \pi^+ & 0 & \gamma_1 \\ v \pi & 0 & \gamma_1 & 0 \end{pmatrix} \begin{pmatrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{pmatrix}$$



# Trigonal warping in bilayer graphene

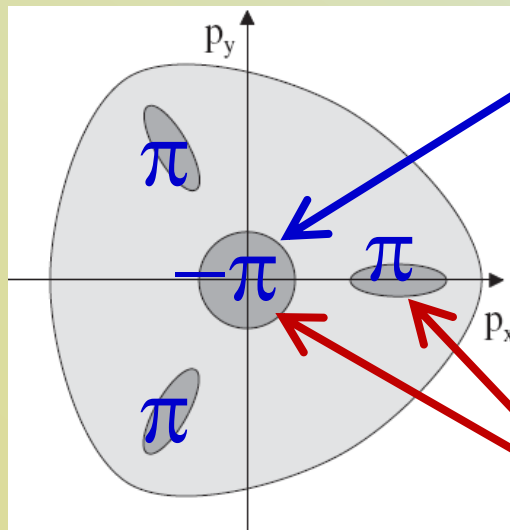
EM and V.I. Fal'ko, PRL **96**, 086805 (2006)

$$H_2 = \frac{-1}{2m} \begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} + v_3 \begin{pmatrix} 0 & \pi \\ \pi^+ & 0 \end{pmatrix} + \dots$$

## Trigonal warping

$$\varepsilon^2 = \left( \frac{p^2}{2m} \right)^2 - \frac{\xi v_3 p^3}{m} \cos 3\phi + v_3^2 p^2$$

Perturbation arising from "skew" interlayer coupling  $v_3 = \frac{\sqrt{3}}{2} a \gamma_3 / \hbar$   
 $\pi = p_x + ip_y$



Dispersion is linear inside each pocket, with chirality corresponding to that of a monolayer

J.L. Manes, F. Guinea, and M.A. Vozmediano, PRB **75**, 155424 (2007);

G.P. Mikitik and Y. Sharlai, PRB **77**, 113407 (2008).

Lifshitz transition:

Fermi surface separation

$$\varepsilon_L \approx \frac{\gamma_1}{4} \left( \frac{v_3}{v} \right)^2 \sim 1 \text{ meV}$$



## Low-energy Hamiltonian of bilayer graphene

EM and V.I. Fal'ko, PRL **96**, 086805 (2006)

$$H_2 = \frac{-1}{2m} \begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} + v_3 \begin{pmatrix} 0 & \pi \\ \pi^+ & 0 \end{pmatrix} + \dots$$

Perturbation arising from “skew” interlayer coupling  $v_3 = \frac{\sqrt{3}}{2} a \gamma_3 / \hbar$   
 $\pi = p_x + ip_y$

## Low-energy Hamiltonian of monolayer graphene

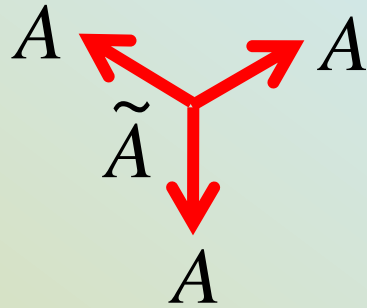
Ajiki and Ando, JPSJ **62**, 2470 (1993)

Ando, Nakanishi, and Saito, JPSJ **67**, 2857 (1998)

$$H_1 = v \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} - \mu \begin{pmatrix} 0 & \pi^2 \\ (\pi^+)^2 & 0 \end{pmatrix} + \dots$$

Perturbation arising from higher-order in momentum expansion

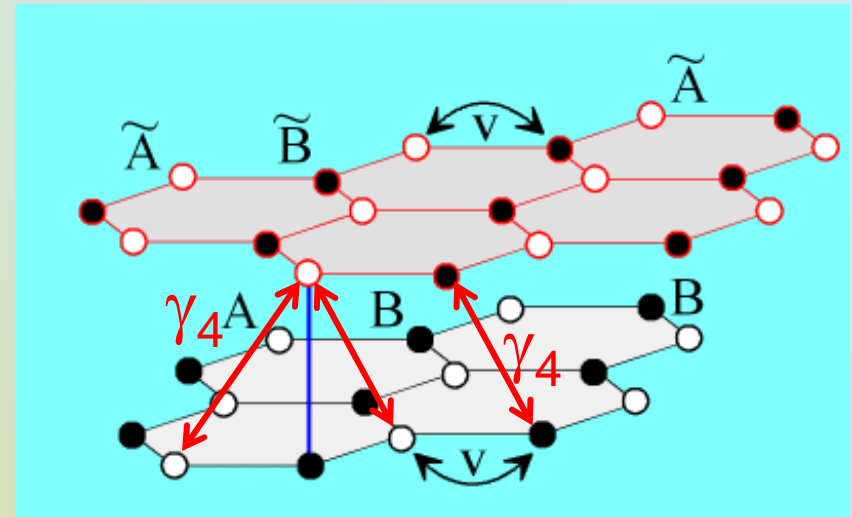
# Role of $\gamma_4$ in bilayer graphene



$$v_4 = \frac{\sqrt{3}}{2} a \gamma_4 / \hbar$$

$$\pi = p_x + ip_y$$

$$H = \begin{pmatrix} A & \tilde{B} & \tilde{A} & B \\ 0 & v_3 \pi & v_4 \pi^+ & v \pi^+ \\ v_3 \pi^+ & 0 & v \pi & v_4 \pi \\ v_4 \pi & v \pi^+ & 0 & \gamma_1 \\ v \pi & v_4 \pi^+ & \gamma_1 & 0 \end{pmatrix} \begin{matrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{matrix}$$



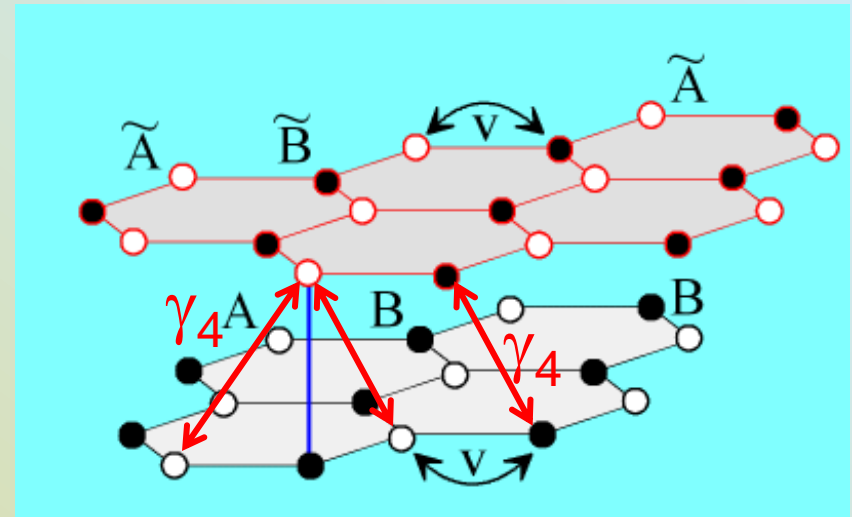
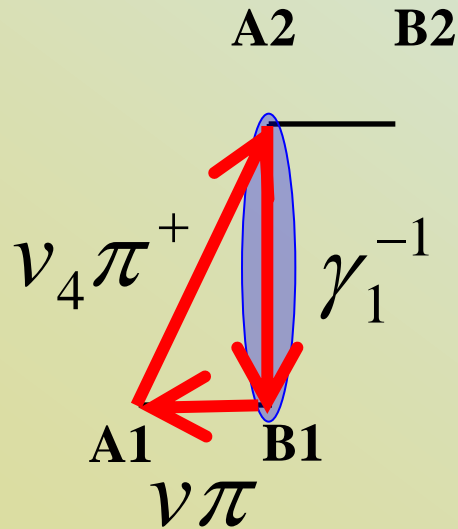
# Role of $\gamma_4$ in bilayer graphene

$$H_2 = \frac{-1}{2m} \begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} + \frac{2v\gamma_4 p^2}{\gamma_1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \dots$$

electron-hole asymmetry arising from "skew" interlayer coupling

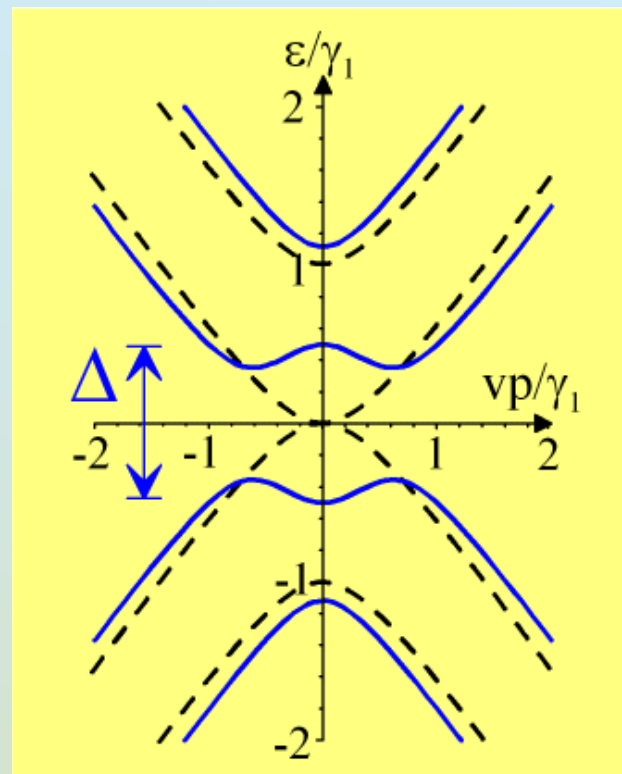
$$v_4 = \frac{\sqrt{3}}{2} a \gamma_4 / \hbar$$

$$\pi = p_x + ip_y$$



# Interlayer asymmetry gap in bilayer graphene

$$H = \begin{pmatrix} A & \tilde{B} & \tilde{A} & B \\ -\Delta/2 & 0 & 0 & v\pi^+ \\ 0 & \Delta/2 & v\pi & 0 \\ 0 & v\pi^+ & \Delta/2 & \gamma_1 \\ v\pi & 0 & \gamma_1 & -\Delta/2 \end{pmatrix} \begin{pmatrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{pmatrix}$$



# Interlayer asymmetry gap in bilayer graphene

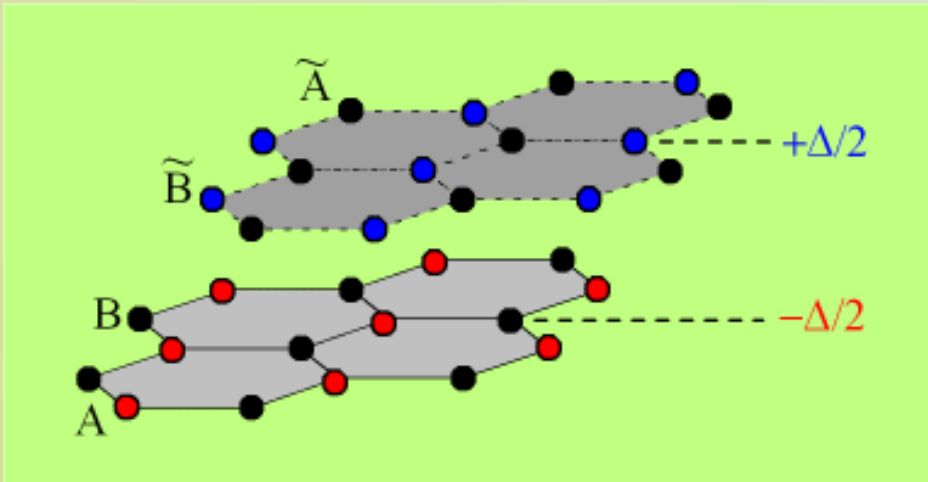
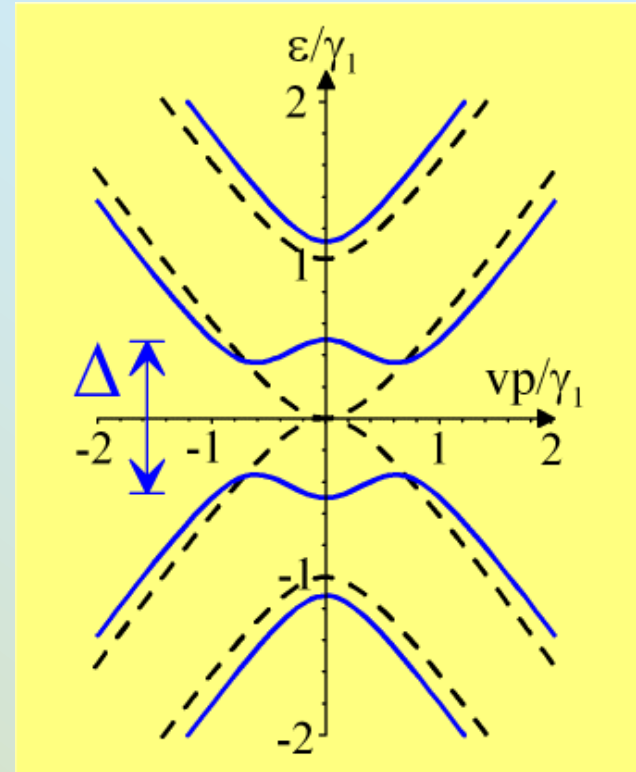
**Bilayer**

**A site;**  
**lower layer**

$$H = \begin{pmatrix} -\Delta/2 & -p^2 e^{-2i\phi} / 2m \\ -p^2 e^{2i\phi} / 2m & \Delta/2 \end{pmatrix}$$

**B site;**  
**upper layer**

$$\Rightarrow E = \pm \sqrt{\frac{\Delta^2}{4} + \left(\frac{p^2}{2m}\right)^2}$$



- EMcC and VI Fal'ko, PRL **96**, 086805 (2006);  
 EMcC, PRB **74**, 161403(R) (2006);  
 H Min, BR Sahu, SK Banerjee, and AH  
 MacDonald, PRB **75**, 155115 (2007);  
 EV Castro *et al*, PRL **99**, 216802 (2007)

## AB-stacked bilayer

$$\hat{H}_{bilayer}^{(eff)} =$$

$$-\frac{v^2}{\gamma_1} \begin{pmatrix} 0 & (p_x - ip_y)^2 \\ (p_x + ip_y)^2 & 0 \end{pmatrix} \quad \text{chirality}$$

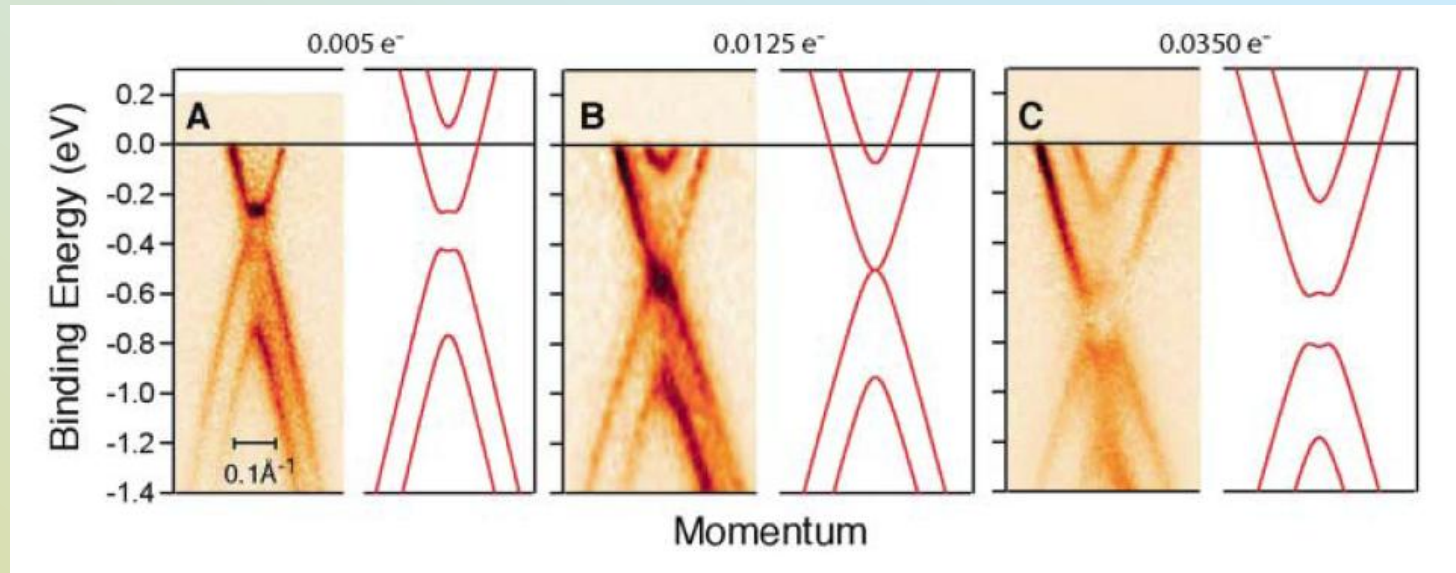
$$+v_3 \begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix} \quad \gamma_3: \text{trigonal warping}$$

$$+\frac{2vv_4 p^2}{\gamma_1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \gamma_4: \text{e-h asymmetry}$$

$$+\Delta \left[ 1 - \frac{2v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{asymmetry gap}$$

This isn't an exhaustive list: e.g. next-nearest neighbours, non-orthogonality, other on-site asymmetry terms, ....

# Interlayer asymmetry gap in bilayer graphene



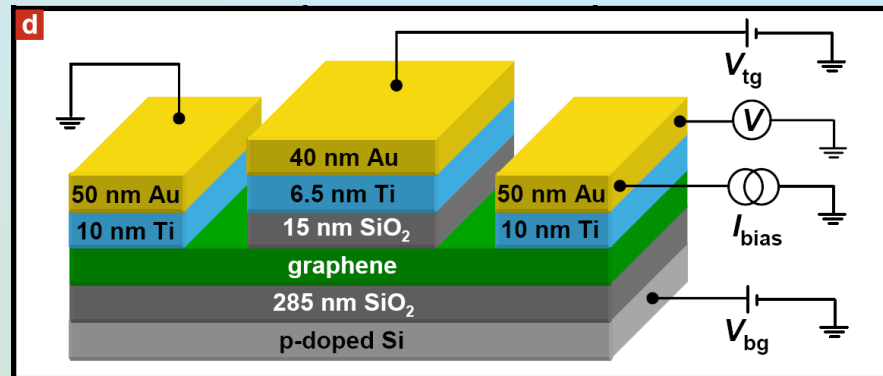
**T Ohta, A Bostwick, T Seyller, K Horn, E Rotenberg,  
Science 313, 951 (2006)**

**Lawrence Berkeley National Lab. (US), Fritz-Haber-Institut and University of Erlangen-Nuremberg (Germany).**

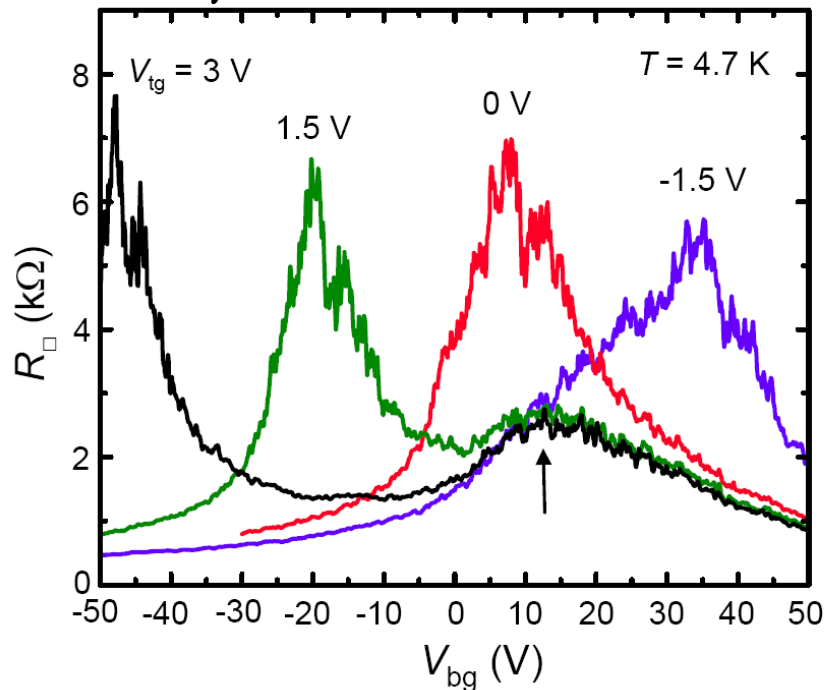
**ARPES measurements of heavily doped bilayer graphene synthesized on a silicon carbide substrate**

# Gate-tunable band-gap in bilayer graphene

JB Oostinga, HB Heersche, X Liu,  
AF Morpurgo, LMK Vandersypen,  
Nature Materials 7, 151 (2007)

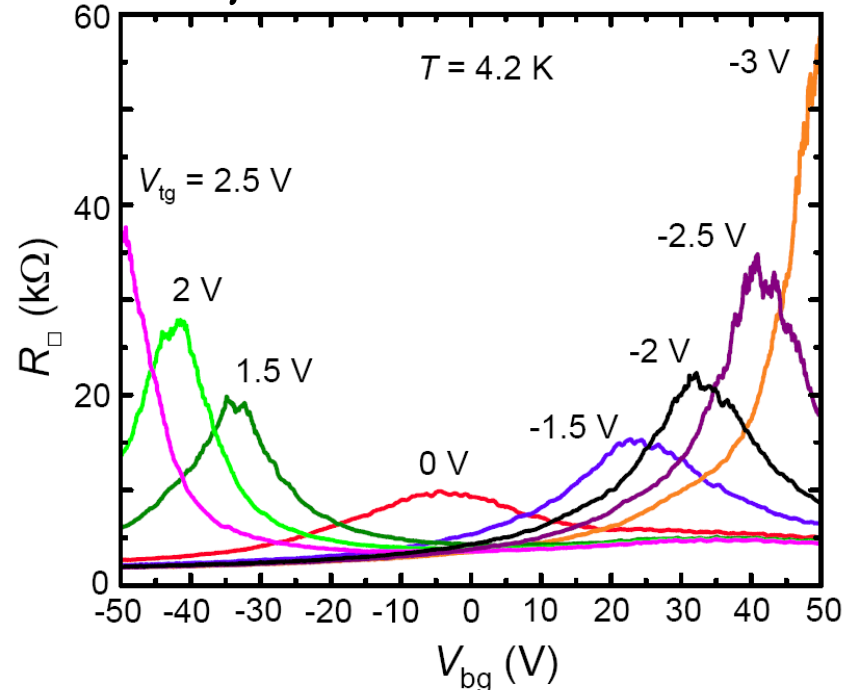


$$\mu \approx 3000 \text{ cm}^2 / \text{Vs}$$



monolayer

$$\mu \approx 1000 \text{ cm}^2 / \text{Vs}$$

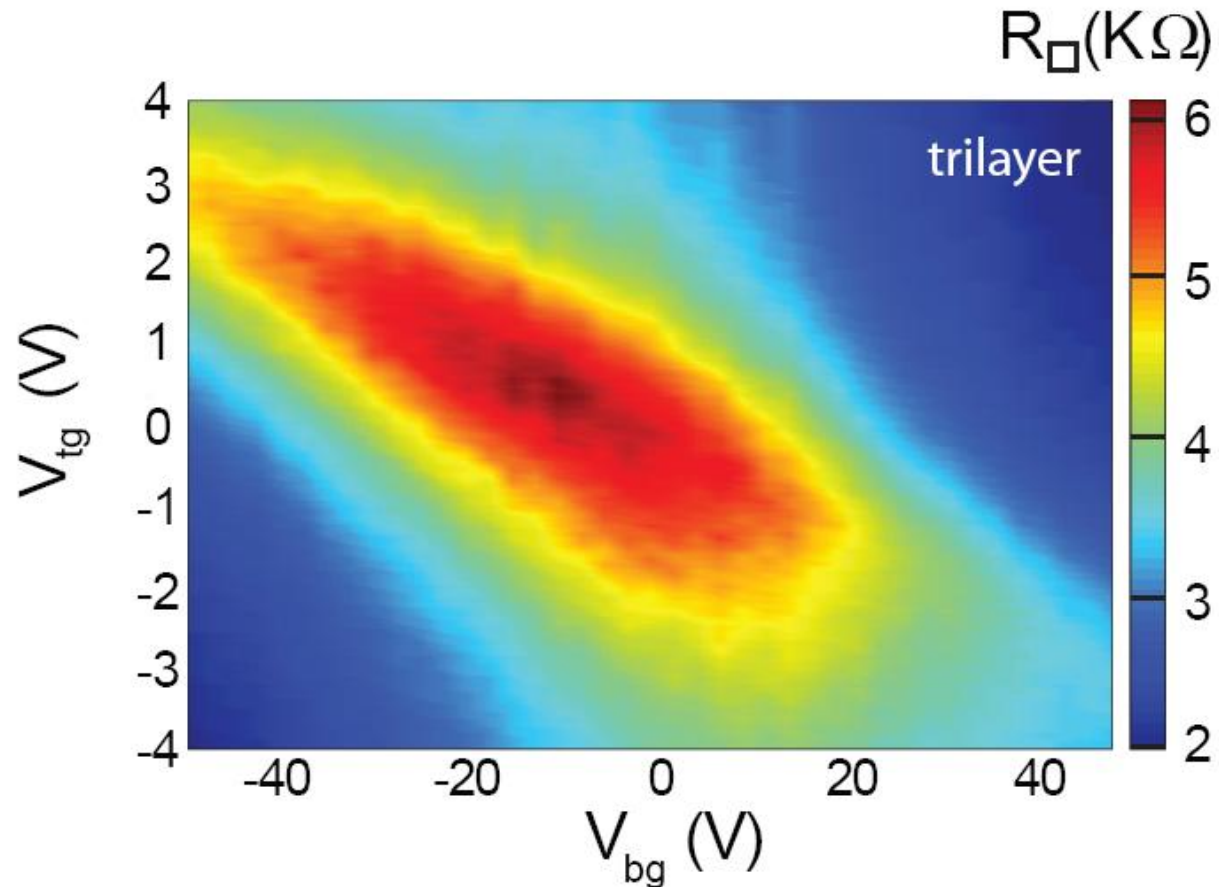
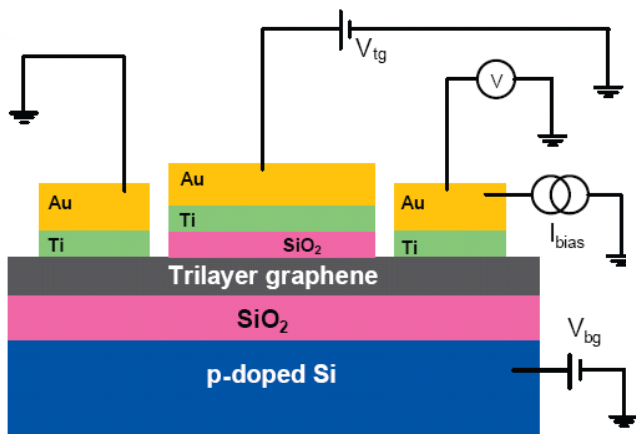
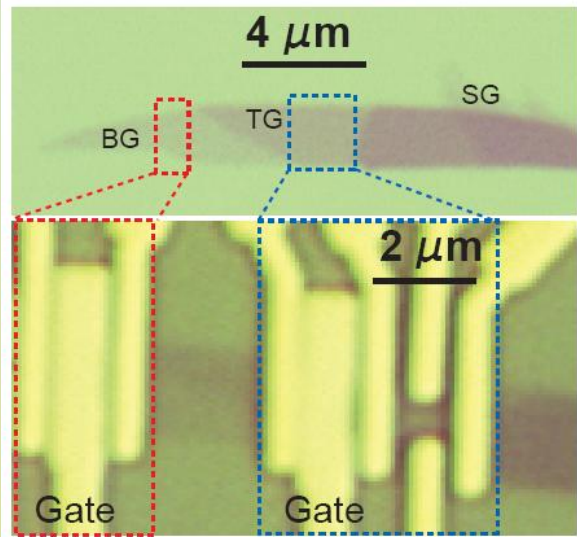


bilayer

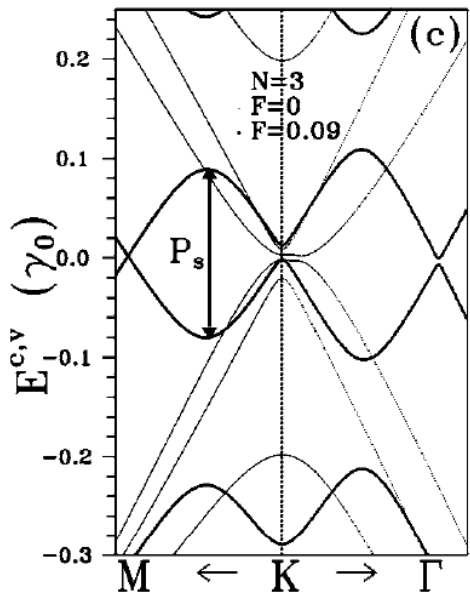
$$E_g \sim 10 \text{ meV}$$



# Trilayer graphene with perpendicular electric field

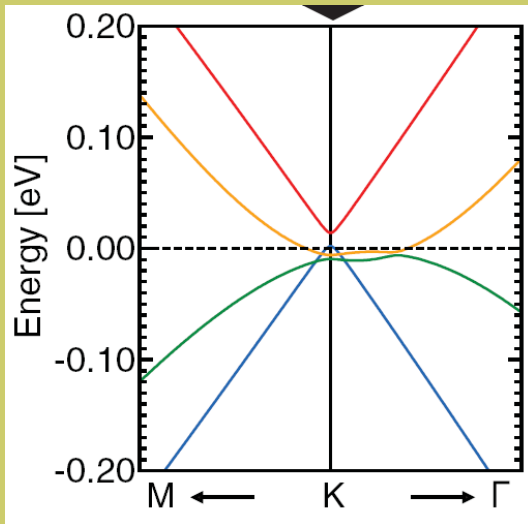


MF Craciun, S Russo, M Yamamoto, JB Oostinga, AF Morpurgo, and S Tarucha, *Nature Nanotech.* **4**, 383 (2009).

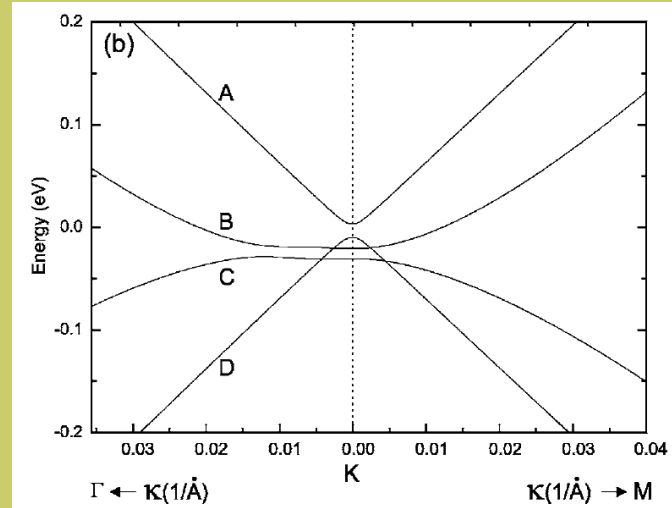


C.L. Lu *et al*, PRB **73**, 144427 (2006)  
**Band gap** (light lines)

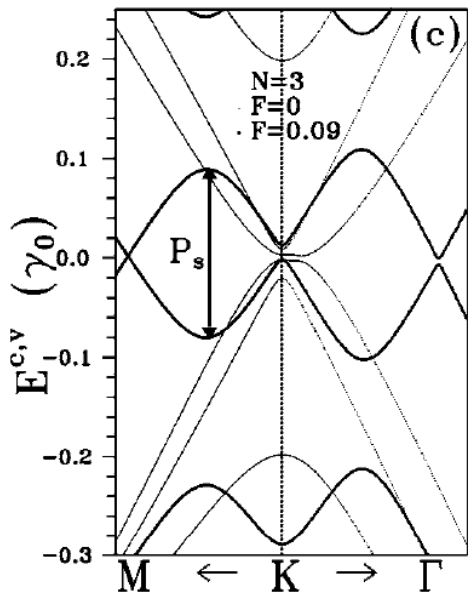
## Theory of band structure of ABA-stacked trilayer graphene



S. Latil and L. Henrard,  
 PRL **97**, 036803 (2006)  
**Band overlap**



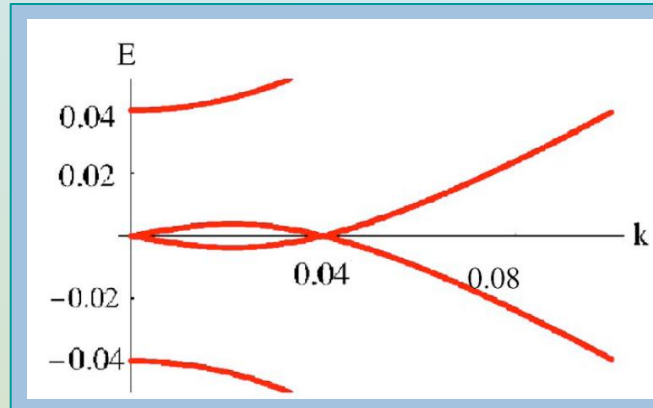
B. Partoens and F.M. Peeters,  
 PRB **74**, 075404 (2006)  
**Band overlap**



C.L. Lu *et al*, PRB **73**, 144427 (2006)

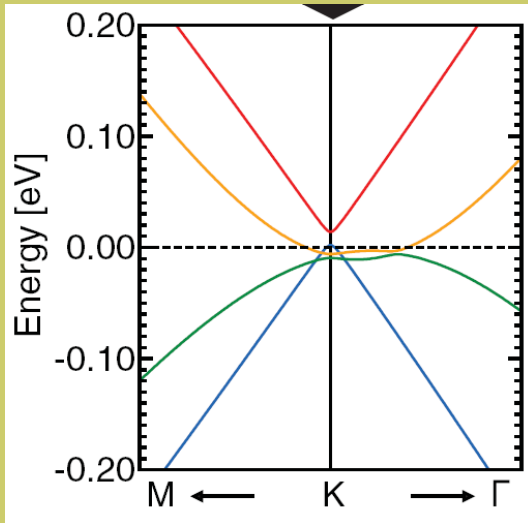
**Band gap** (light lines) for no electric field

Electric field (bold lines) causes crossing and anti-crossing



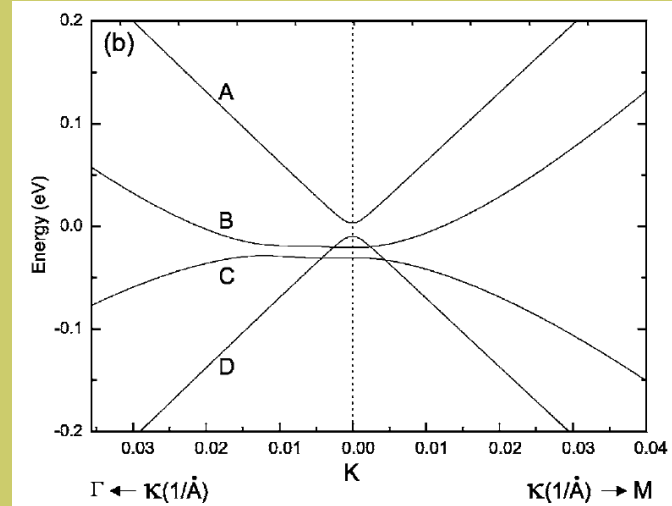
F. Guinea *et al*, PRB **73**, 245426 (2006)

Low energy bands in an electrostatic field



S. Latil and L. Henrard,  
PRL **97**, 036803 (2006)

**Band overlap**

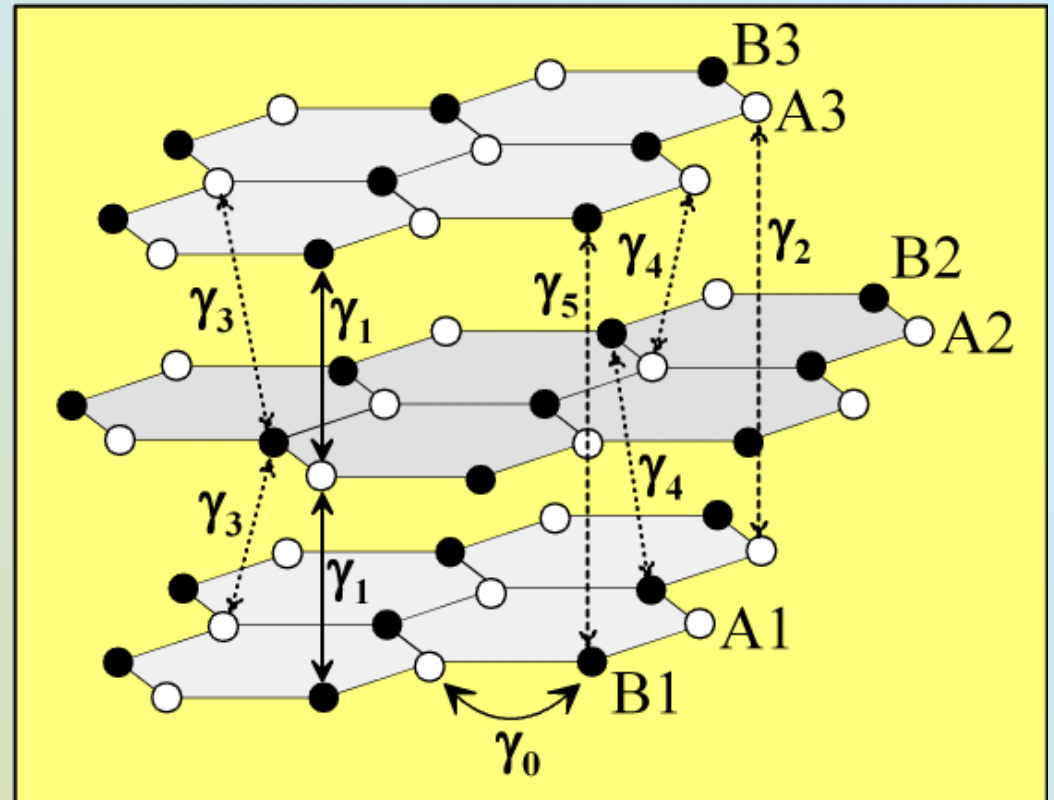
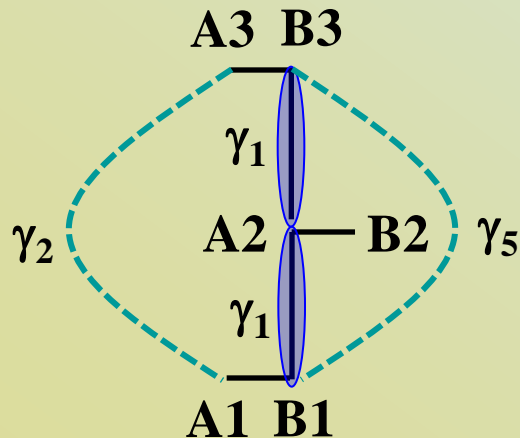


B. Partoens and F.M. Peeters,  
PRB **74**, 075404 (2006)

**Band overlap**

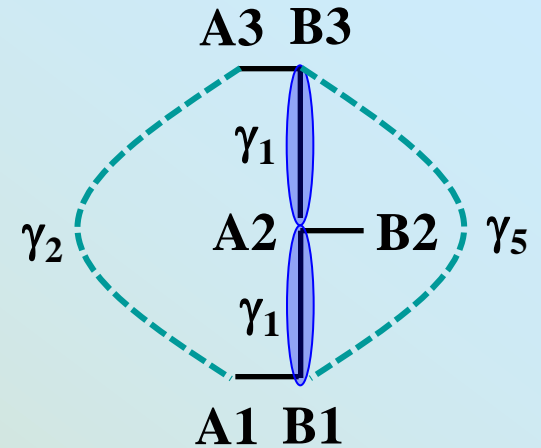
# ABA-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2, \gamma_5$



# ABA-stacked trilayer graphene: tight-binding model

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- Next-nearest layer  $\gamma_2, \gamma_5$

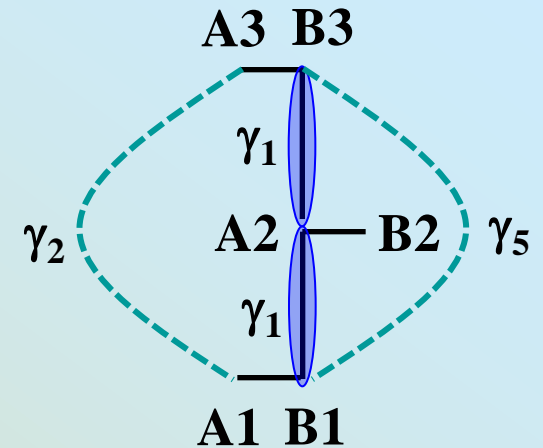


$$\tilde{H} = \begin{pmatrix}
 \mathbf{A1} & \mathbf{B1} & \mathbf{A2} & \mathbf{B2} & \mathbf{A3} & \mathbf{B3} \\
 \begin{pmatrix}
 0 & v\pi^+ & v_4\pi^+ & v_3\pi & \gamma_2 & 0 \\
 v\pi & 0 & \gamma_1 & v_4\pi^+ & 0 & \gamma_5 \\
 v_4\pi & \gamma_1 & 0 & v\pi^+ & v_4\pi & \gamma_1 \\
 v_3\pi^+ & v_4\pi & v\pi & 0 & v_3\pi^+ & v_4\pi \\
 \gamma_2 & 0 & v_4\pi^+ & v_3\pi & 0 & v\pi^+ \\
 0 & \gamma_5 & \gamma_1 & v_4\pi^+ & v\pi & 0
 \end{pmatrix} & \mathbf{A1} \\
 & \mathbf{B1} \\
 & \mathbf{A2} \\
 & \mathbf{B2} \\
 & \mathbf{A3} \\
 & \mathbf{B3}
 \end{pmatrix}$$

$$\begin{aligned}
 \pi &= p_x + ip_y \\
 v &= \frac{\sqrt{3}}{2} a\gamma_0 / \hbar \\
 v_3 &= \frac{\sqrt{3}}{2} a\gamma_3 / \hbar \\
 v_4 &= \frac{\sqrt{3}}{2} a\gamma_4 / \hbar
 \end{aligned}$$

# ABA-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2, \gamma_5$



$$\tilde{H} = \begin{pmatrix} \text{A1} & \text{B1} & \text{A2} & \text{B2} & \text{A3} & \text{B3} \\ \begin{matrix} 0 & v\pi^+ & v_4\pi^+ & v_3\pi & \gamma_2 & 0 \\ v\pi & 0 & \gamma_1 & v_4\pi^+ & 0 & \gamma_5 \\ v_4\pi & \gamma_1 & 0 & v\pi^+ & v_4\pi & \gamma_1 \\ v_3\pi^+ & v_4\pi & v\pi & 0 & v_3\pi^+ & v_4\pi \\ \gamma_2 & 0 & v_4\pi^+ & v_3\pi & 0 & v\pi^+ \\ 0 & \gamma_5 & \gamma_1 & v_4\pi^+ & v\pi & 0 \end{matrix} \end{pmatrix}$$

**A1** Couplings  $\gamma_0, \gamma_3, \gamma_4$  all occur between 3 nearest neighbours so appear linear in small momentum  $p$

**B1**

**A2**

**B2**

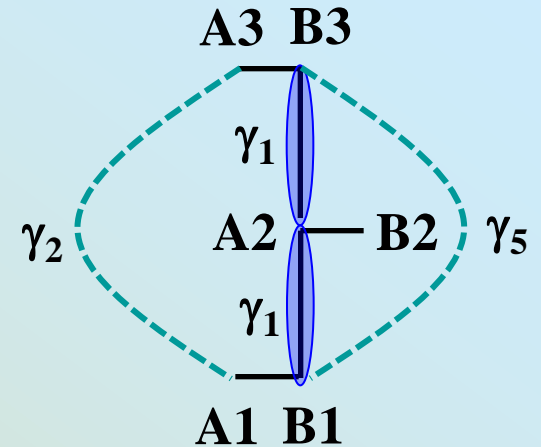
**A3**

**B3**



# ABA-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2, \gamma_5$

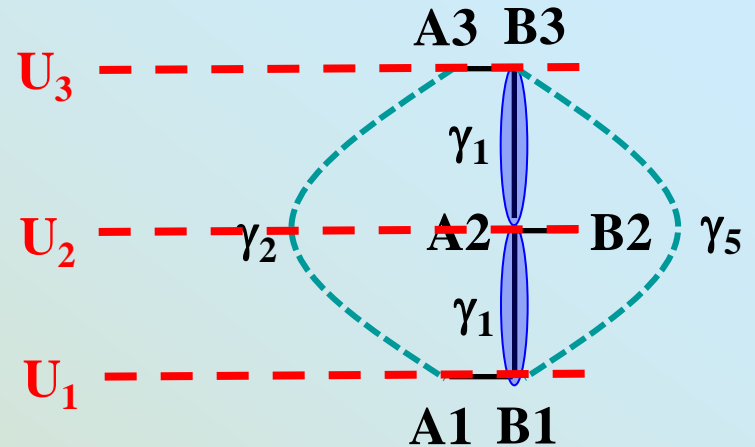


$$\tilde{H} = \begin{pmatrix}
 \text{A1} & \text{B1} & \text{A2} & \text{B2} & \text{A3} & \text{B3} \\
 0 & v\pi^+ & v_4\pi^+ & v_3\pi & \gamma_2 & 0 \\
 v\pi & 0 & \gamma_1 & v_4\pi^+ & 0 & \gamma_5 \\
 v_4\pi & \gamma_1 & 0 & v\pi^+ & v_4\pi & \gamma_1 \\
 v_3\pi^+ & v_4\pi & v\pi & 0 & v_3\pi^+ & v_4\pi \\
 \gamma_2 & 0 & v_4\pi^+ & v_3\pi & 0 & v\pi^+ \\
 0 & \gamma_5 & \gamma_1 & v_4\pi^+ & v\pi & 0
 \end{pmatrix}$$

**A1** Couplings  $\gamma_1, \gamma_2, \gamma_5$  are vertical (with only 1 partner) so are independent of small momentum  $p$   
**B1**  
**A2**  
**B2**  
**A3**  
**B3**

# ABA-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2, \gamma_5$
- Interlayer asymmetry  $U_1, U_2, U_3$



$$\tilde{H} = \begin{pmatrix} U_1 & v\pi^+ & v_4\pi^+ & v_3\pi & \gamma_2 & 0 \\ v\pi & U_1 & \gamma_1 & v_4\pi^+ & 0 & \gamma_5 \\ v_4\pi & \gamma_1 & U_2 & v\pi^+ & v_4\pi & \gamma_1 \\ v_3\pi^+ & v_4\pi & v\pi & U_2 & v_3\pi^+ & v_4\pi \\ \gamma_2 & 0 & v_4\pi^+ & v_3\pi & U_3 & v\pi^+ \\ 0 & \gamma_5 & \gamma_1 & v_4\pi^+ & v\pi & U_3 \end{pmatrix} \begin{matrix} \mathbf{A1} \\ \mathbf{B1} \\ \mathbf{A2} \\ \mathbf{B2} \\ \mathbf{A3} \\ \mathbf{B3} \end{matrix}$$



# ABA-stacked trilayer graphene: mirror-reflection symmetry

Introduce new basis:

$$\phi_1 = (A1 - A3) / \sqrt{2} \quad \text{odd}$$

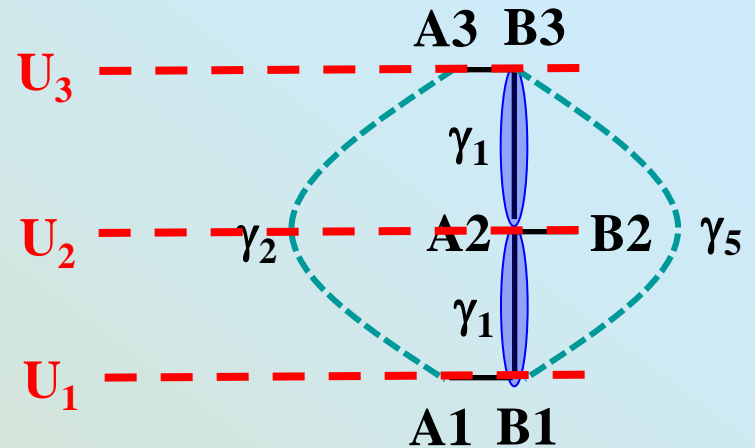
$$\phi_2 = (B1 - B3) / \sqrt{2} \quad \text{odd}$$

$$\phi_3 = (A1 + A3) / \sqrt{2} \quad \text{even}$$

$$\phi_4 = B2 \quad \text{even}$$

$$\phi_5 = A2 \quad \text{even}$$

$$\phi_6 = (B1 + B3) / \sqrt{2} \quad \text{even}$$



Introduce new asymmetry parameters:

$$\Delta_1 = (U_1 - U_3) / 2 \quad \text{odd} \quad \text{asymmetry between outer layers}$$

$$\Delta_2 = (U_1 - 2U_2 + U_3) / 6 \quad \text{even} \quad \text{central layer is at different energy to the (average of the) outer ones}$$

$$U_1 + U_2 + U_3 = 0 \quad \text{average energy is zero}$$

# ABA-stacked trilayer graphene: mirror-reflection symmetry

Monolayer block (odd)

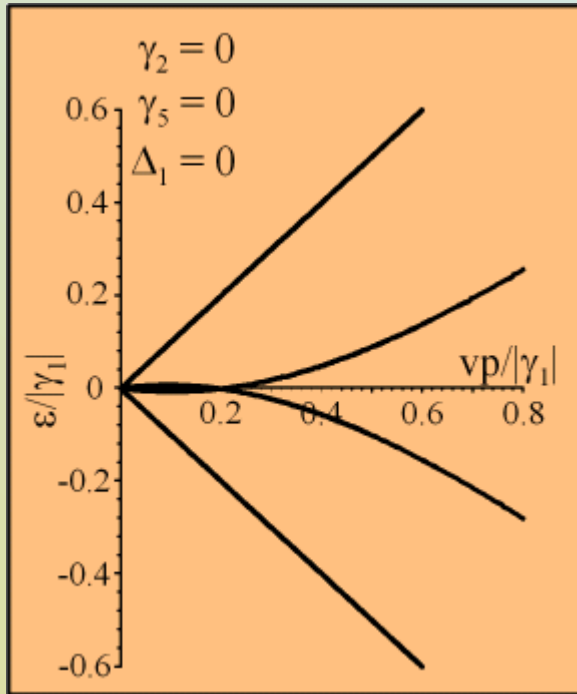
$\Delta_2, \gamma_2, \gamma_5$  only appear on main diagonal

$$H = \begin{pmatrix} \Delta_2 - \gamma_2 & v\pi^+ & \Delta_1 & 0 & 0 & 0 \\ v\pi & \Delta_2 - \gamma_5 & 0 & 0 & 0 & \Delta_1 \\ \Delta_1 & 0 & \Delta_2 + \gamma_2 & \sqrt{2}v_3\pi & \sqrt{2}v_4\pi^+ & v\pi^+ \\ 0 & 0 & \sqrt{2}v_3\pi^+ & -2\Delta_2 & v\pi & \sqrt{2}v_4\pi \\ 0 & 0 & \sqrt{2}v_4\pi & v\pi^+ & -2\Delta_2 & \sqrt{2}\gamma_1 \\ 0 & \Delta_1 & v\pi & \sqrt{2}v_4\pi^+ & \sqrt{2}\gamma_1 & \Delta_2 + \gamma_5 \end{pmatrix}$$

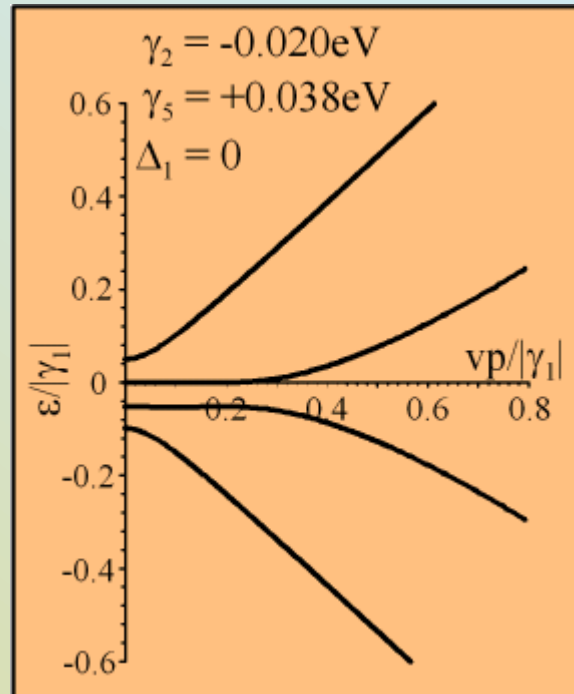
$\pi = p_x + ip_y$

Bilayer block (even)

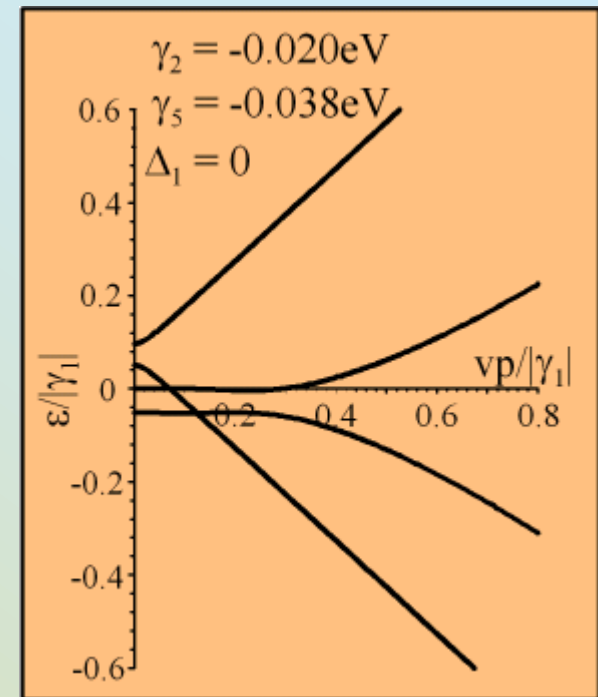
# ABA-stacked trilayer graphene: next-nearest layer coupling



separate monolayer  
and bilayer bands  
(2 each at low energy,  
plus 2 bilayer bands at  
 $\pm \sqrt{2} \gamma_1$ )



$\gamma_2, \gamma_5$  shift the  
monolayer and  
bilayer bands...  
to produce a gap



or an overlap

# ABA-stacked trilayer graphene: mirror-reflection symmetry

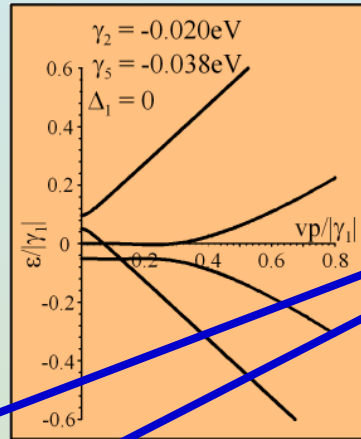
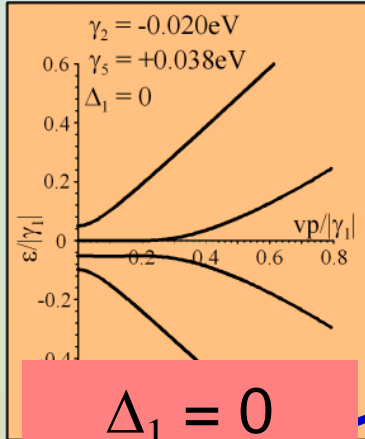
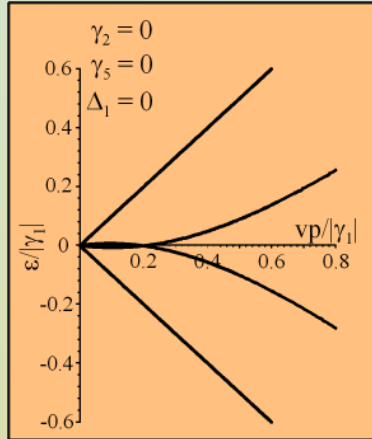
Monolayer block (odd)

$$H = \begin{pmatrix} \Delta_2 - \gamma_2 & v\pi^+ & \Delta_1 & 0 & 0 & 0 \\ v\pi & \Delta_2 - \gamma_5 & 0 & 0 & 0 & \Delta_1 \\ \Delta_1 & 0 & \Delta_2 + \gamma_2 & \sqrt{2}v_3\pi & \sqrt{2}v_4\pi^+ & v\pi^+ \\ 0 & 0 & \sqrt{2}v_3\pi^+ & -2\Delta_2 & v\pi & \sqrt{2}v_4\pi \\ 0 & 0 & \sqrt{2}v_4\pi & v\pi^+ & -2\Delta_2 & \sqrt{2}\gamma_1 \\ 0 & \Delta_1 & v\pi & \sqrt{2}v_4\pi^+ & \sqrt{2}\gamma_1 & \Delta_2 + \gamma_5 \end{pmatrix}$$

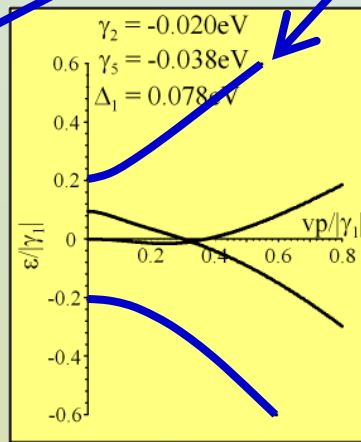
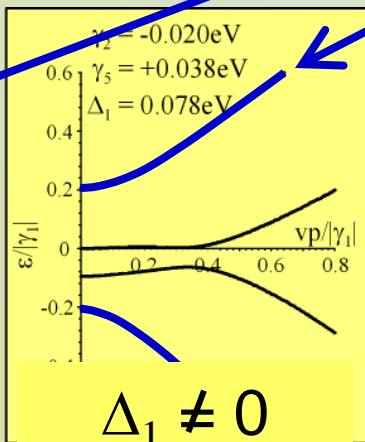
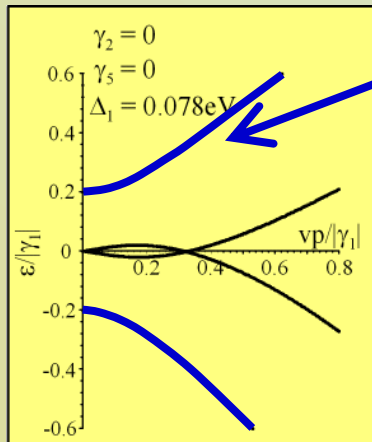
$\Delta_1$  is the only parameter to break mirror reflection symmetry so it can appear in the off-diagonal block

Bilayer block (even)

# ABA-stacked trilayer graphene: mirror-reflection symmetry



- $\Delta_1$  mixes monolayer and bilayer bands
- 2 bands go to energy  $\pm \Delta_1$

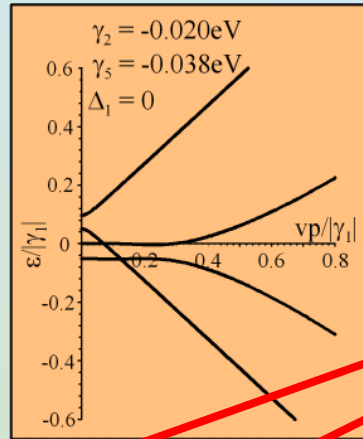
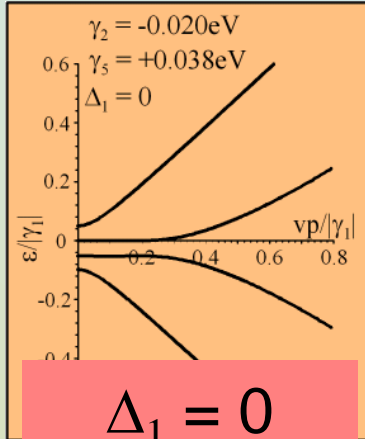
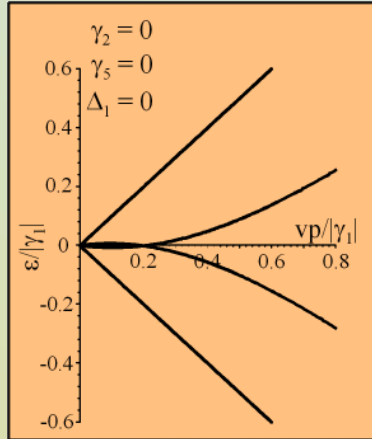


$\gamma_2 = \gamma_5 = 0$

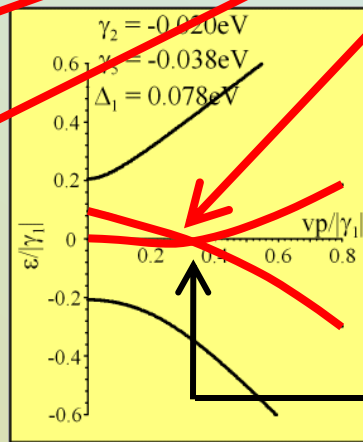
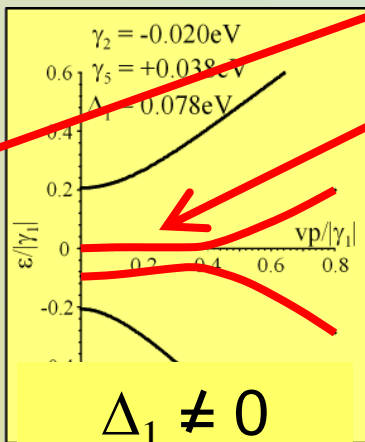
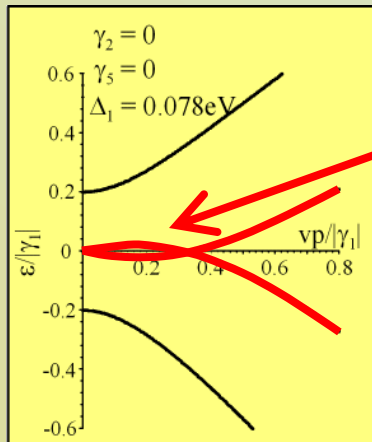
$\text{sign}(\gamma_2) = -\text{sign}(\gamma_5)$

$\text{sign}(\gamma_2) = +\text{sign}(\gamma_5)$

# ABA-stacked trilayer graphene: mirror-reflection symmetry



- $\Delta_1$  mixes monolayer and bilayer bands
- 2 bands go to energy  $\pm \Delta_1$
- 2 bands stay near zero energy



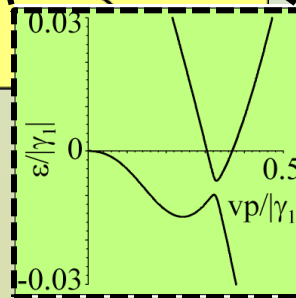
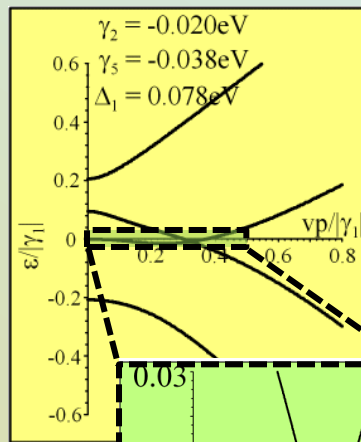
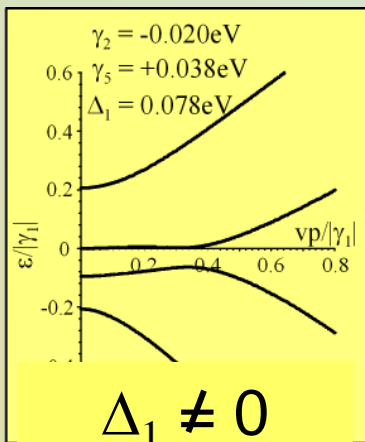
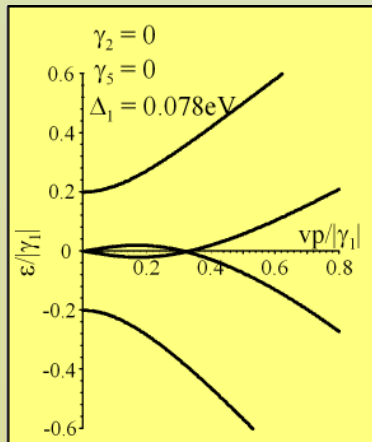
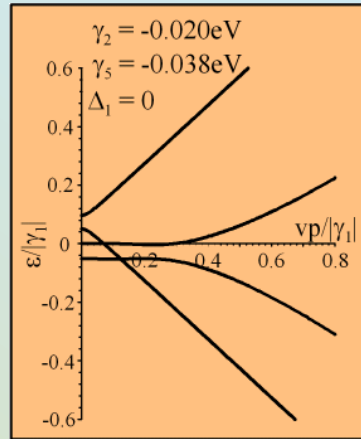
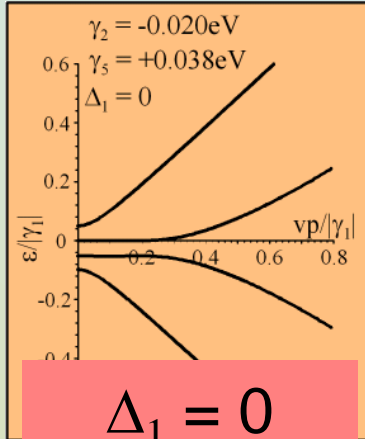
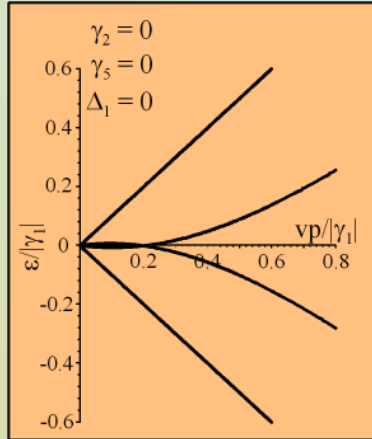
anticrossing near  
momentum  $p \approx \Delta_1 / v$

$\gamma_2 = \gamma_5 = 0$

$\text{sign}(\gamma_2) =$   
 $- \text{sign}(\gamma_5)$

$\text{sign}(\gamma_2) =$   
 $+ \text{sign}(\gamma_5)$

# ABA-stacked trilayer graphene: mirror-reflection symmetry



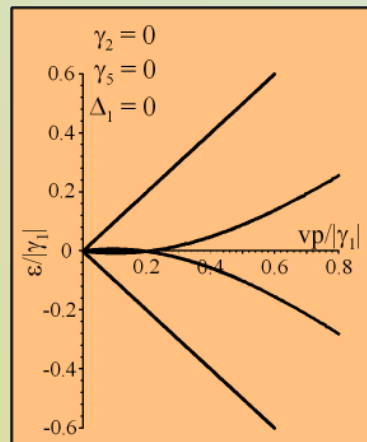
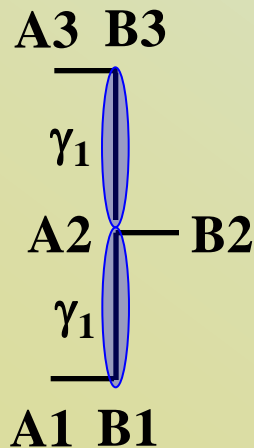
- $\Delta_1$  mixes monolayer and bilayer bands
- 2 bands go to energy  $\pm \Delta_1$
- 2 bands stay near zero energy with anti-crossing at momentum  $p \approx \Delta_1 / v$
- size of hybridization gap is  $\sim |\gamma_2 - \gamma_5| / 2$

Unlike bilayer, the gap doesn't grow with  $\Delta_1$ , only the position of the anticrossing  $p \sim \Delta_1 / v$

# ABA-stacked trilayer graphene: low-energy effective Hamiltonian #1

$$H = \begin{pmatrix} 0 & v\pi^+ & \Delta_1 & 0 & 0 & 0 \\ v\pi & 0 & 0 & 0 & 0 & \Delta_1 \\ \Delta_1 & 0 & 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & 0 & 0 & v\pi & 0 \\ 0 & 0 & 0 & v\pi^+ & 0 & \sqrt{2}\gamma_1 \\ 0 & \Delta_1 & v\pi & 0 & \sqrt{2}\gamma_1 & 0 \end{pmatrix}$$

$\pi = p_x + ip_y$



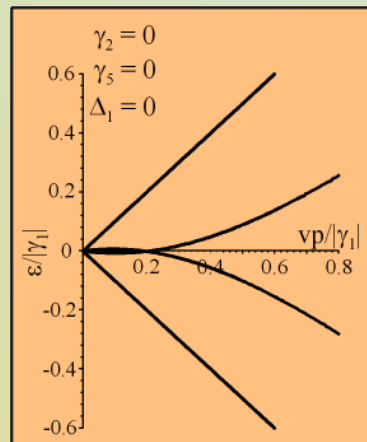
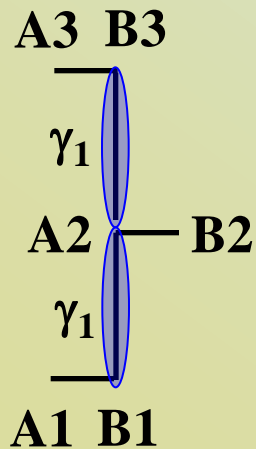
Let's simplify things by  
keeping only  $v$ ,  $\gamma_1$  and  $\Delta_1$ .



# ABA-stacked trilayer graphene: low-energy effective Hamiltonian #1

$$H = \begin{pmatrix} 0 & v\pi^+ & \Delta_1 & 0 & 0 & 0 \\ v\pi & 0 & 0 & 0 & 0 & \Delta_1 \\ \Delta_1 & 0 & 0 & 0 & 0 & v\pi^+ \\ 0 & 0 & 0 & 0 & v\pi & 0 \\ 0 & 0 & 0 & v\pi^+ & 0 & \sqrt{2}\gamma_1 \\ 0 & \Delta_1 & v\pi & 0 & \sqrt{2}\gamma_1 & 0 \end{pmatrix}$$

$\pi = p_x + ip_y$

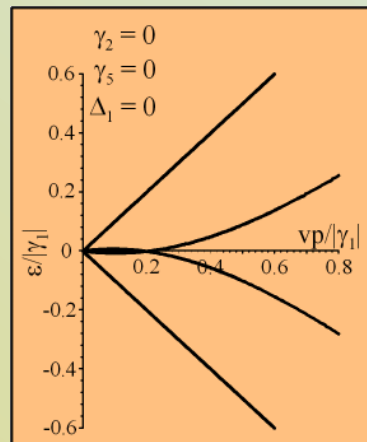
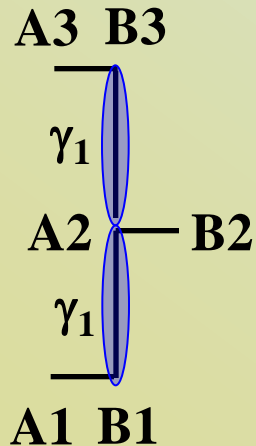


There are four bands near zero energy (at  $\varepsilon \ll \gamma_1$ ) so we can eliminate the “high-energy” bilayer components:  $\phi_5 = A2$

$$\phi_6 = (B1 + B3) / \sqrt{2}$$

# ABA-stacked trilayer graphene: low-energy effective Hamiltonian #1

$$H = \begin{pmatrix} \begin{array}{cc|cc} 0 & v\pi^+ & \Delta_1 & 0 \\ v\pi & 0 & 0 & -\frac{\Delta_1 v\pi^+}{\sqrt{2}\gamma_1} \\ \hline \Delta_1 & 0 & 0 & -\frac{(v\pi^+)^2}{\sqrt{2}\gamma_1} \\ 0 & -\frac{\Delta_1 v\pi}{\sqrt{2}\gamma_1} & -\frac{(v\pi)^2}{\sqrt{2}\gamma_1} & 0 \end{array} \end{pmatrix}$$

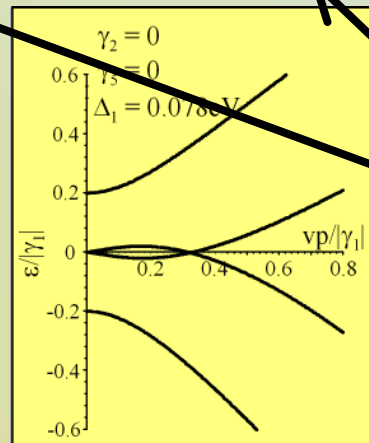
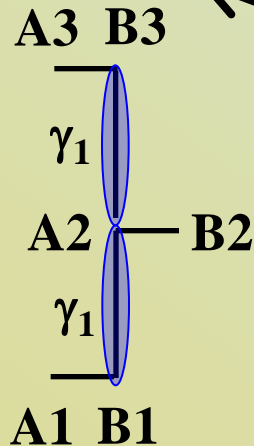


Effective Hamiltonian describing  
four bands near zero energy  
(at  $\epsilon \ll \gamma_1$ )

# ABA-stacked trilayer graphene:

## low-energy effective Hamiltonian #2: large $\Delta_1$

$$H = \begin{pmatrix} 0 & v\pi^+ & \Delta_1 & 0 \\ v\pi & 0 & 0 & -\frac{\Delta_1 v\pi^+}{\sqrt{2}\gamma_1} \\ \Delta_1 & 0 & 0 & -\frac{(v\pi^+)^2}{\sqrt{2}\gamma_1} \\ 0 & -\frac{\Delta_1 v\pi}{\sqrt{2}\gamma_1} & -\frac{(v\pi)^2}{\sqrt{2}\gamma_1} & 0 \end{pmatrix}$$



For large  $\Delta_1$  there are two bands near zero energy (at  $\epsilon \ll \Delta_1 \ll \gamma_1$ ) so we can eliminate another two components:  $\phi_1 = (A1 - A3)/\sqrt{2}$   
 $\phi_3 = (A1 + A3)/\sqrt{2}$

# ABA-stacked trilayer graphene:

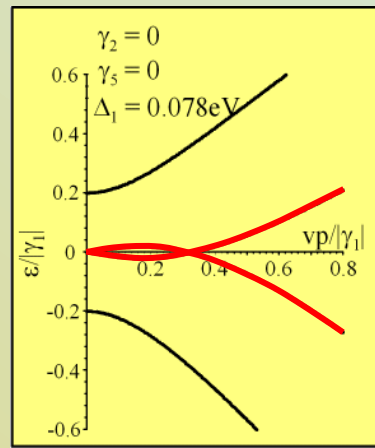
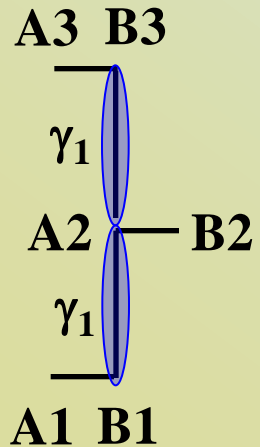
## low-energy effective Hamiltonian #2: large $\Delta_1$

$$H = \begin{pmatrix} 0 & -\left(1 + \frac{v^2 \pi \pi^+}{\Delta_1^2}\right)^{-1/2} \left(1 - \frac{v^2 \pi \pi^+}{\Delta_1^2}\right) \frac{\Delta_1 v \pi^+}{\sqrt{2} \gamma_1} \\ \frac{\Delta_1 v \pi}{\sqrt{2} \gamma_1} \left(1 - \frac{v^2 \pi \pi^+}{\Delta_1^2}\right) \left(1 + \frac{v^2 \pi \pi^+}{\Delta_1^2}\right)^{-1/2} & 0 \end{pmatrix}$$

in basis of  $\phi_2 = (B1 - B3)/\sqrt{2}$  and  $\phi_4 = B2$

chiral quasiparticles even for large asymmetry

$$\psi = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi/2} \\ \mp e^{+i\phi/2} \end{pmatrix}$$



For large  $\Delta_1$  there are two bands near zero energy (at  $\epsilon \ll \Delta_1 \ll \gamma_1$ ).

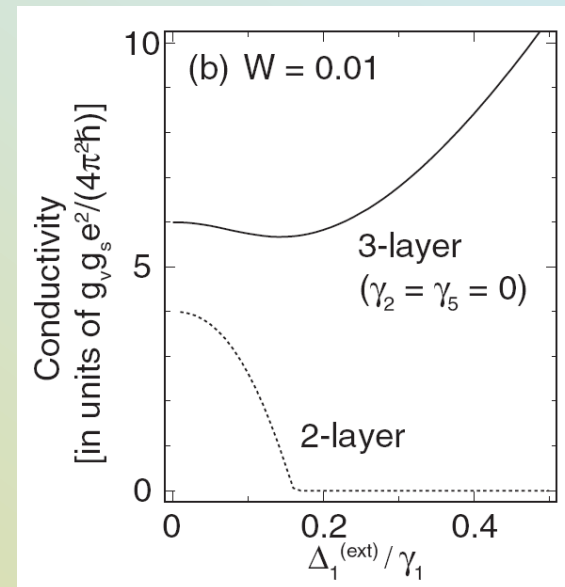
$$\gamma_2 = \gamma_3 = \gamma_4 = \gamma_5 = \Delta_2 = 0$$

$$\epsilon \approx \pm \frac{vp}{\sqrt{2} \gamma_1} \frac{(v^2 p^2 - \Delta_1^2)}{\sqrt{v^2 p^2 + \Delta_1^2}}$$

# Summary of ABA-trilayer

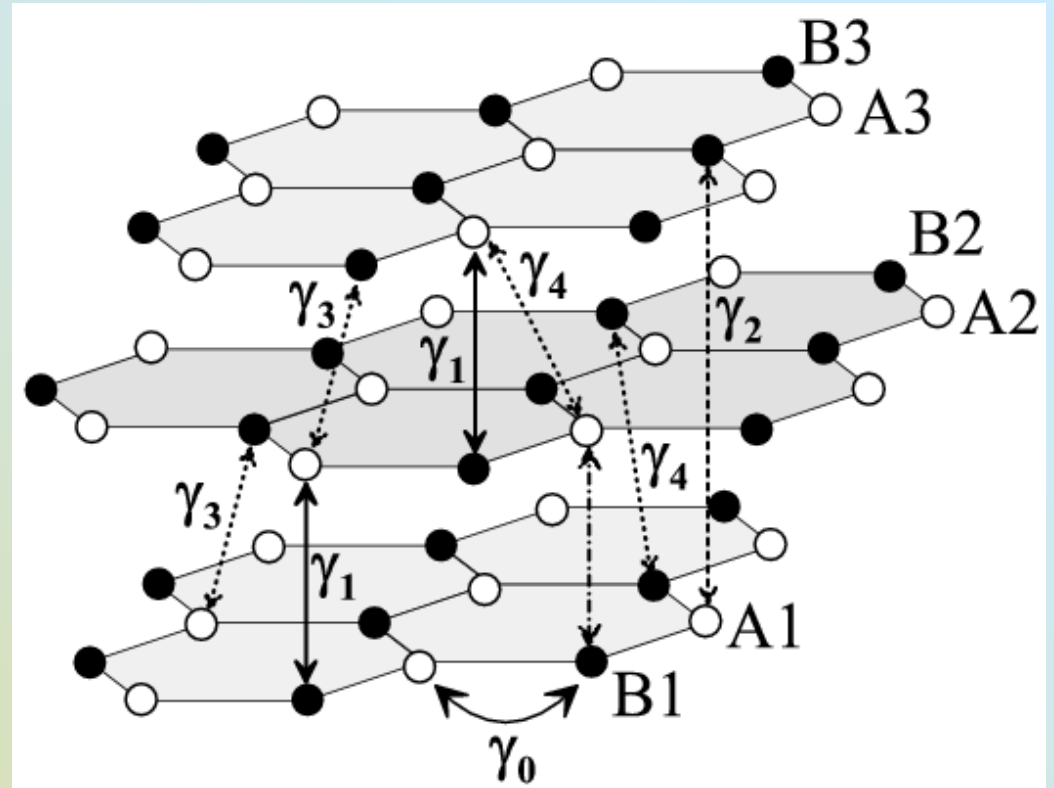
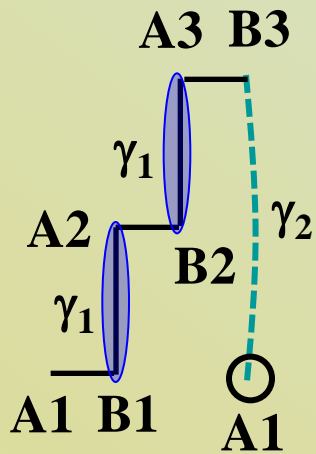
- ABA-stacked trilayer graphene:
  - Interlayer asymmetry  $\Delta_1$  hybridises low-energy linear and parabolic bands
  - Two low-energy bands with an anti-crossing and gap  $\ll \Delta_1$
  - The bands still support chiral quasiparticles
  - Density of states and minimal conductivity increase with  $\Delta_1$

Mikito Koshino and E McCann, Phys Rev B **79**, 125443 (2009).



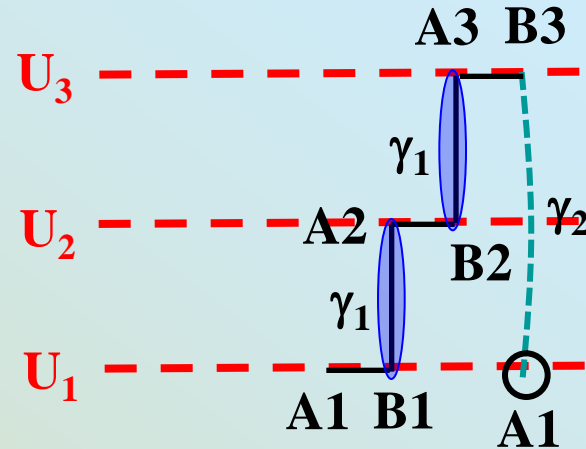
# ABC-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2$



# ABC-stacked trilayer graphene: tight-binding model

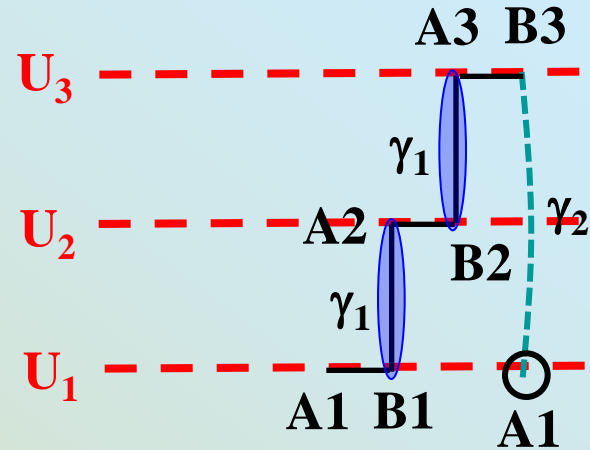
- 3 layers of carbon atoms
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(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2$
- Interlayer asymmetry  $U_1, U_2, U_3$



$$H = \begin{pmatrix} U_1 & v\pi^+ & v_4\pi^+ & v_3\pi & 0 & \gamma_2/2 \\ v\pi & U_1 & \gamma_1 & v_4\pi^+ & 0 & 0 \\ v_4\pi & \gamma_1 & U_2 & v\pi^+ & v_4\pi^+ & v_3\pi \\ v_3\pi^+ & v_4\pi & v\pi & U_2 & \gamma_1 & v_4\pi^+ \\ 0 & 0 & v_4\pi & \gamma_1 & U_3 & v\pi^+ \\ \gamma_2/2 & 0 & v_3\pi^+ & v_4\pi & v\pi & U_3 \end{pmatrix} \begin{matrix} \mathbf{A1} \\ \mathbf{B1} \\ \mathbf{A2} \\ \mathbf{B2} \\ \mathbf{A3} \\ \mathbf{B3} \end{matrix}$$

# ABC-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2$
- Interlayer asymmetry  $U_1, U_2, U_3$



$$H = \begin{pmatrix} A1 & B1 & A2 & B2 & A3 & B3 \\ U_1 & v\pi^+ & v_4\pi^+ & v_3\pi & 0 & \gamma_2/2 \\ v\pi & U_1 & \gamma_1 & v_4\pi^+ & 0 & 0 \\ v_4\pi & \gamma_1 & U_2 & v\pi^+ & v_4\pi^+ & v_3\pi \\ v_3\pi^+ & v_4\pi & v\pi & U_2 & \gamma_1 & v_4\pi^+ \\ 0 & 0 & v_4\pi & \gamma_1 & U_3 & v\pi^+ \\ \gamma_2/2 & 0 & v_3\pi^+ & v_4\pi & v\pi & U_3 \end{pmatrix}$$

**A1** Couplings  $\gamma_0, \gamma_3, \gamma_4$  all occur between 3 nearest neighbours so appear linear in small momentum  $p$

**B1**

**A2**

**B2**

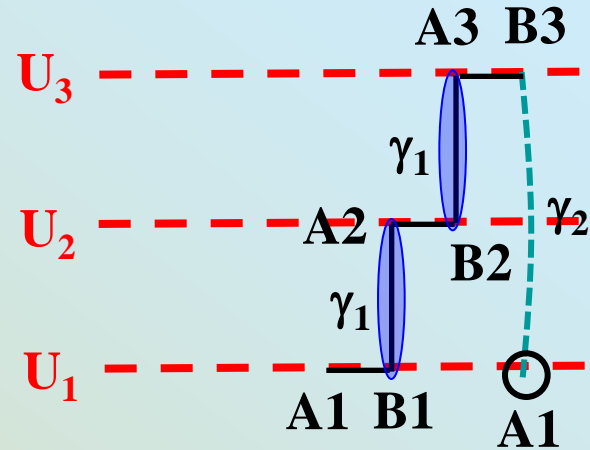
**A3**

**B3**



# ABC-stacked trilayer graphene: tight-binding model

- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2$
- Interlayer asymmetry  $U_1, U_2, U_3$

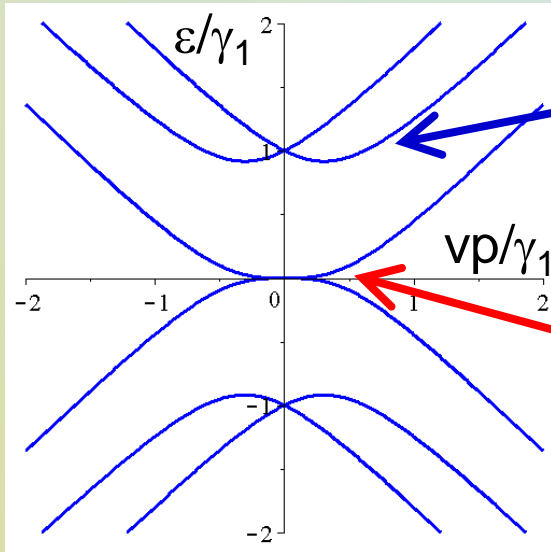


$$H = \begin{pmatrix} U_1 & v\pi^+ & v_4\pi^+ & v_3\pi & 0 & \gamma_2/2 \\ v\pi & U_1 & \gamma_1 & v_4\pi^+ & 0 & 0 \\ v_4\pi & \gamma_1 & U_2 & v\pi^+ & v_4\pi^+ & v_3\pi \\ v_3\pi^+ & v_4\pi & v\pi & U_2 & \gamma_1 & v_4\pi^+ \\ 0 & 0 & v_4\pi & \gamma_1 & U_3 & v\pi^+ \\ \gamma_2/2 & 0 & v_3\pi^+ & v_4\pi & v\pi & U_3 \end{pmatrix}$$

**A1** Couplings  $\gamma_1$ , and  $\gamma_2$   
**B1** are vertical (with  
**A2** only 1 partner) so  
**B2** are independent of  
**A3** small momentum  $p$   
**B3**

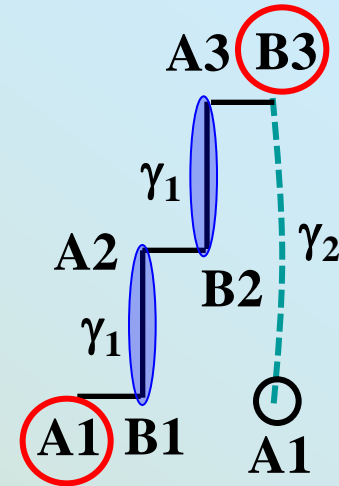
# ABC-stacked trilayer graphene: tight-binding model

$$\gamma_2 = \gamma_3 = \gamma_4 = U_1 = U_2 = U_3 = 0$$



high-energy bands  
created by B1A2 and  
B2A3 dimers

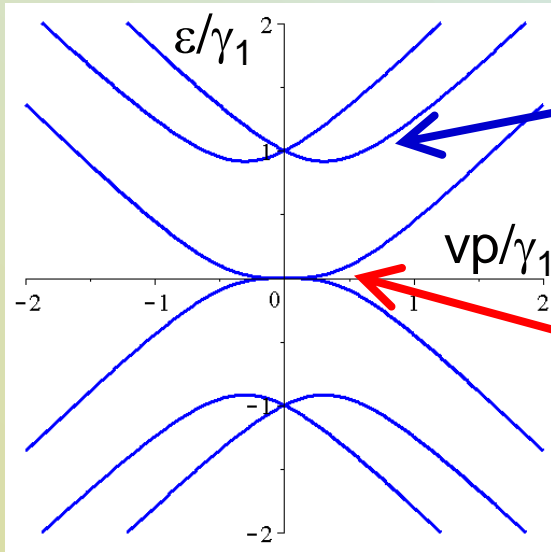
low-energy bands  
created by effective  
hopping A1 to B3:  
cubic generalisation of  
bilayer bands



- F. Guinea *et al*, PRB **73**, 245426 (2006);  
 S. Latil and L. Henrard, PRL **97**, 036803 (2006);  
 C.-L. Lu *et al*, APL **89**, 221910 (2006);  
 M. Aoki and H. Amawashi, SSC **142**, 123 (2007).

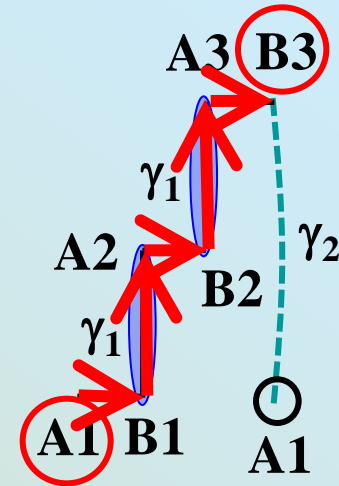
# ABC-stacked trilayer graphene: tight-binding model

$$\gamma_2 = \gamma_3 = \gamma_4 = U_1 = U_2 = U_3 = 0$$



high-energy bands  
created by B1A2 and  
B2A3 dimers

low-energy bands  
created by effective  
hopping A1 to B3:  
cubic generalisation of  
bilayer bands



$$\hat{H}_{ABC}^{(eff)} = \frac{v^3}{\gamma_1^2} \begin{pmatrix} 0 & (p_x - ip_y)^3 \\ (p_x + ip_y)^3 & 0 \end{pmatrix}$$

chirality related to  
Berry's phase  $3\pi$

- F. Guinea *et al*, PRB **73**, 245426 (2006);  
 J.L. Manes, F. Guinea, and M.A. Vozmediano, PRB **75**, 155424 (2007);  
 H. Min and A.H. MacDonald, PRB **77**, 155416 (2008).

## AB-stacked bilayer

$$\hat{H}_{bilayer}^{(eff)} =$$

$$-\frac{v^2}{\gamma_1} \begin{pmatrix} 0 & (p_x - ip_y)^2 \\ (p_x + ip_y)^2 & 0 \end{pmatrix} \quad \text{chirality}$$

$$+v_3 \begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix} \quad \text{trigonal warping}$$

$$+\frac{2vv_4 p^2}{\gamma_1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \gamma_4: \text{e-h asymmetry}$$

$$+\Delta \left[ 1 - \frac{2v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{asymmetry gap}$$

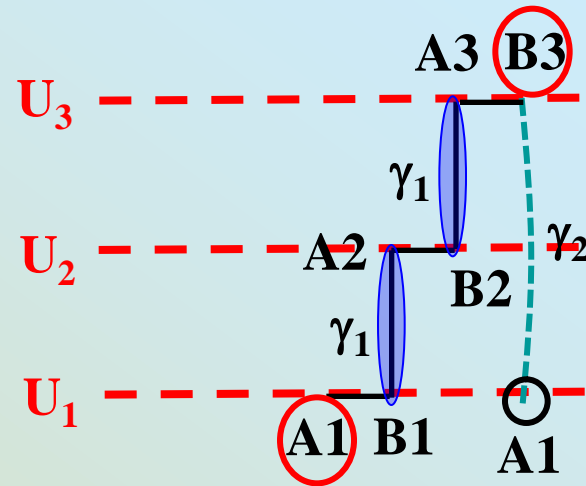
## ABC-stacked trilayer

$$\hat{H}_{ABC}^{(eff)} =$$

$$\frac{v^3}{\gamma_1^2} \begin{pmatrix} 0 & (p_x - ip_y)^3 \\ (p_x + ip_y)^3 & 0 \end{pmatrix}$$

# ABC-stacked trilayer graphene: interlayer asymmetry

- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2$
- Interlayer asymmetry  $U_1, U_2, U_3$



New asymmetry parameters:

$$\Delta_1 = (U_1 - U_3)/2$$

$$\Delta_2 = (U_1 - 2U_2 + U_3)/6$$

breaks symmetry  
between A1 and B3  
sites, opening a gap

$$\Delta_1 \left[ 1 - \frac{v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

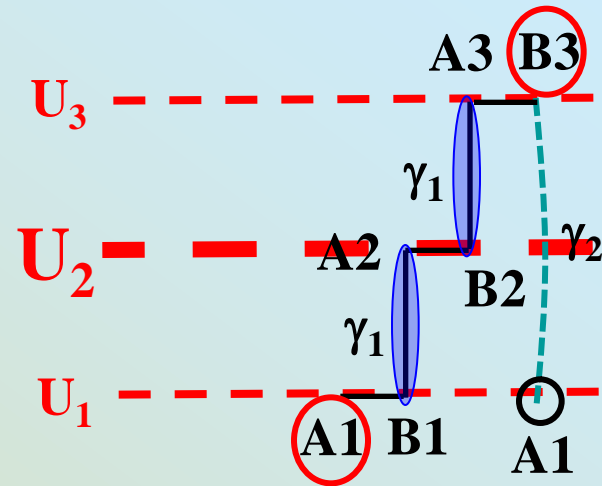
in A1/B3 basis

F. Guinea *et al*, PRB **73**, 245426 (2006);

M. Aoki and H. Amawashi, SSC **142**, 123 (2007).

# ABC-stacked trilayer graphene: interlayer asymmetry

- 3 layers of carbon atoms
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- Next-nearest layer  $\gamma_2$
- Interlayer asymmetry  $U_1, U_2, U_3$



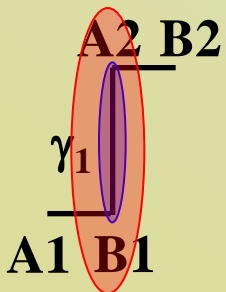
New asymmetry parameters:

$$\Delta_1 = (U_1 - U_3)/2$$

$$\Delta_2 = (U_1 - 2U_2 + U_3)/6$$

The central layer is at a different potential to the outer layers: it introduces e-h asymmetry

$$\Delta_2 \begin{bmatrix} 1 - \frac{3v^2 p^2}{\gamma_1^2} & \\ & \end{bmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



In a bilayer, a similar term is produced by asymmetry between the dimer (B1A2) and non-dimer sites (A1B2)

$$\Delta_{\text{graphite}} \begin{bmatrix} 1 - \frac{2v^2 p^2}{\gamma_1^2} & \\ & \end{bmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

## AB-stacked bilayer

$$\hat{H}_{bilayer}^{(eff)} =$$

$$-\frac{v^2}{\gamma_1} \begin{pmatrix} 0 & (p_x - ip_y)^2 \\ (p_x + ip_y)^2 & 0 \end{pmatrix} \quad \text{chirality}$$

$$+v_3 \begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix} \quad \text{trigonal warping}$$

$$+\frac{2vv_4 p^2}{\gamma_1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \gamma_4: \text{e-h asymmetry}$$

$$+\Delta \left[ 1 - \frac{2v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{asymmetry gap}$$

$$+\Delta_{graphite} \left[ 1 - \frac{2v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{more e-h asymmetry}$$

## ABC-stacked trilayer

$$\hat{H}_{ABC}^{(eff)} =$$

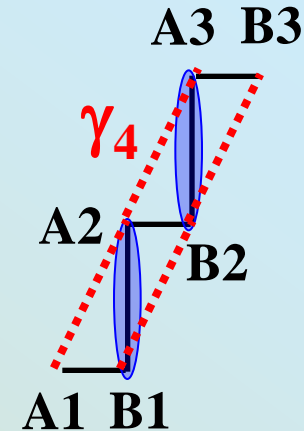
$$\frac{v^3}{\gamma_1^2} \begin{pmatrix} 0 & (p_x - ip_y)^3 \\ (p_x + ip_y)^3 & 0 \end{pmatrix}$$

$$+\Delta_1 \left[ 1 - \frac{v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$+\Delta_2 \left[ 1 - \frac{3v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

# ABC-stacked trilayer graphene: role of $\gamma_4$

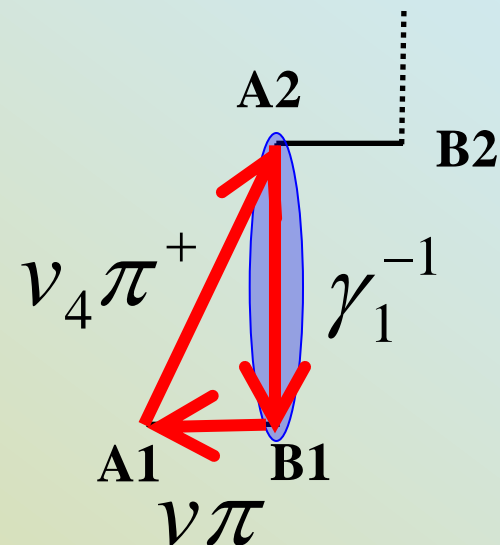
- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- **Interlayer coupling**  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2$
- Interlayer asymmetry  $U_1, U_2, U_3$



It creates the same term in the effective Hamiltonian as for the bilayer, describing electron-hole asymmetry

$$\frac{2v v_4 p^2}{\gamma_1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

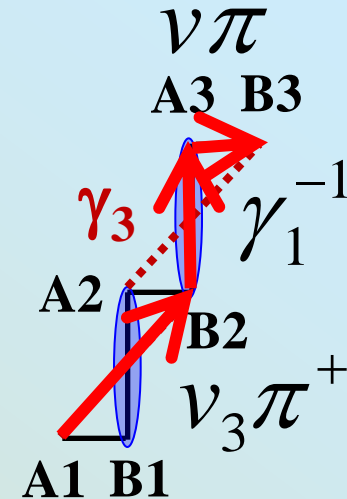
This term only involves the outer two layers, so it will have the same form in all N-layer ABC multilayers ( $N > 1$ ).





# ABC-stacked trilayer graphene: role of $\gamma_3$

- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1,B1,A2,B2,A3,B3)
- Hopping within a layer  $\gamma_0$
- **Interlayer coupling**  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2$
- Interlayer asymmetry  $U_1, U_2, U_3$

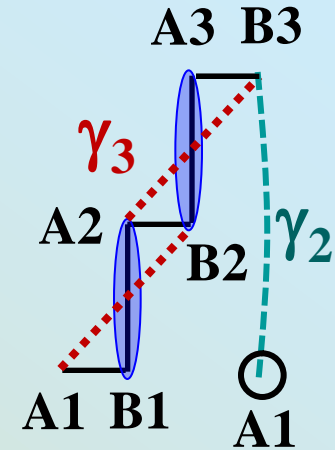


“skew” interlayer coupling  $\gamma_3$   
contributes to trigonal warping

$$-\frac{2vv_3p^2}{\gamma_1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

# ABC-stacked trilayer graphene: role of $\gamma_3$ and $\gamma_2$

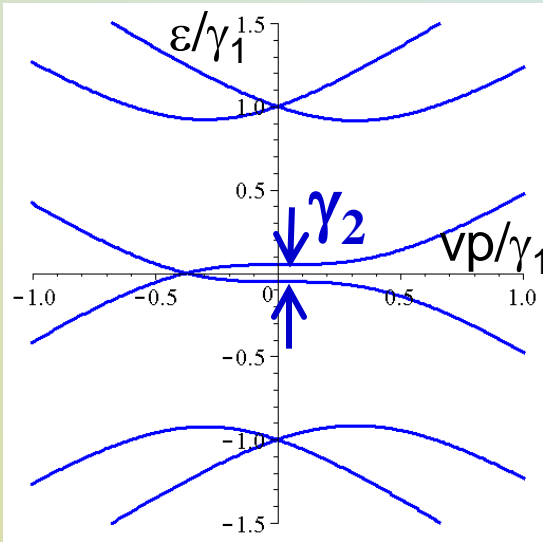
- 3 layers of carbon atoms
- 6 atoms in the unit cell  
(A1, B1, A2, B2, A3, B3)
- Hopping within a layer  $\gamma_0$
- Interlayer coupling  $\gamma_1, \gamma_3, \gamma_4$
- Next-nearest layer  $\gamma_2$
- Interlayer asymmetry  $U_1, U_2, U_3$



“skew” interlayer coupling  $\gamma_3$   
contributes to trigonal warping  $-\frac{2vv_3p^2}{\gamma_1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

vertical, next-nearest layer coupling  
 $\gamma_2$  contributes to trigonal warping  $\frac{\gamma_2}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

# ABC-stacked trilayer graphene: role of $\gamma_3$ and $\gamma_2$



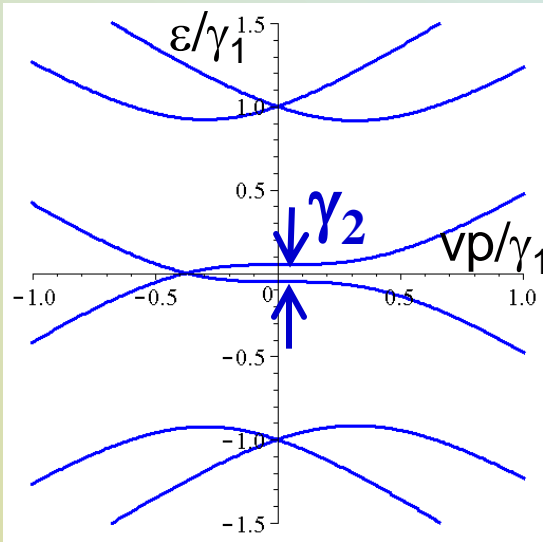
Even though coupling  $\gamma_2$  may be small ( $|\gamma_2| \sim 20\text{meV}$ ?), the  $\gamma_2$  term is important because it doesn't vanish at the K point.

S. Latil and L. Henrard, PRL **97**, 036803 (2006);  
C.-L. Lu *et al*, APL **89**, 221910 (2006);  
M. Aoki and H. Amawashi, SSC **142**, 123 (2007).

“skew” interlayer coupling  $\gamma_3$   
contributes to trigonal warping  $-\frac{2vv_3p^2}{\gamma_1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

vertical, next-nearest layer coupling  
 $\gamma_2$  contributes to trigonal warping  $\frac{\gamma_2}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

# ABC-stacked trilayer graphene: role of $\gamma_3$ and $\gamma_2$



Even though coupling  $\gamma_2$  may be small ( $|\gamma_2| \sim 20\text{meV}$ ), the  $\gamma_2$  term is important because it doesn't vanish at the K point.

It sets the energy scale for the Lifshitz transition:

$$\varepsilon_L \approx \frac{\gamma_2}{2} \sim 10\text{meV}$$

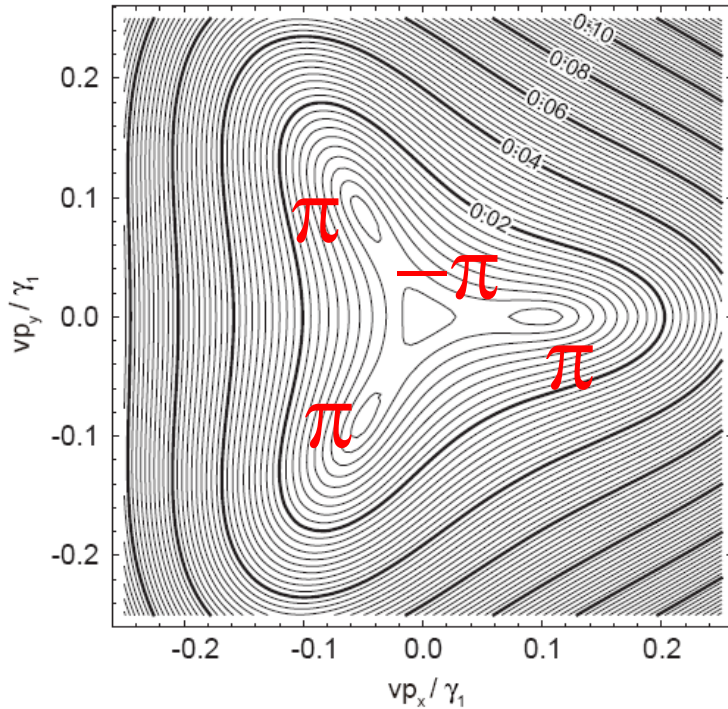
cf. bilayer 
$$\varepsilon_L \approx \frac{\gamma_1}{4} \left( \frac{v_3}{v} \right)^2 \sim 1\text{meV}$$

“skew” interlayer coupling  $\gamma_3$  contributes to trigonal warping 
$$-\frac{2vv_3p^2}{\gamma_1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

vertical, next-nearest layer coupling  $\gamma_2$  contributes to trigonal warping 
$$\frac{\gamma_2}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

# Trigonal warping and Berry's phase

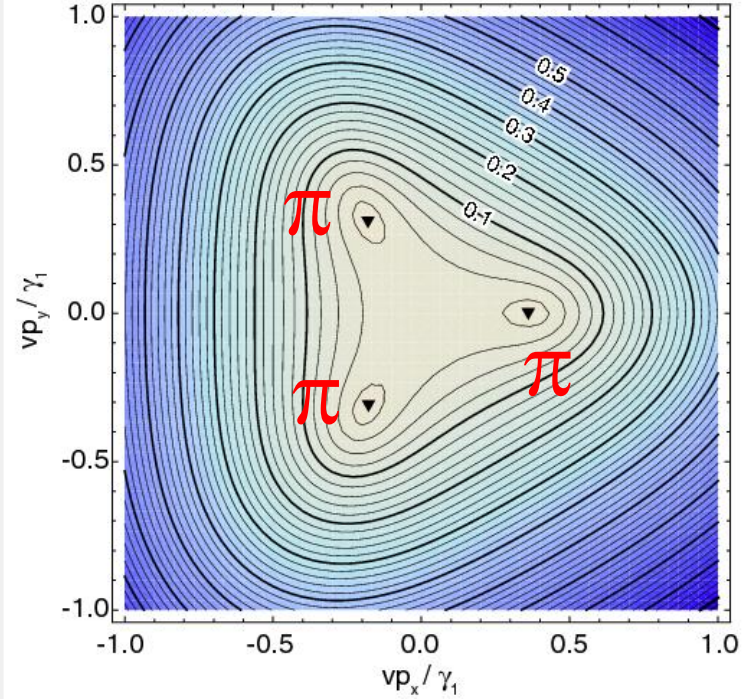
bilayer  
Berry's phase  $2\pi$



central pocket

$$\varepsilon_L \approx \frac{\gamma_1}{4} \left( \frac{v_3}{v} \right)^2 \sim 1 \text{ meV}$$

ABC-trilayer  
Berry's phase  $3\pi$

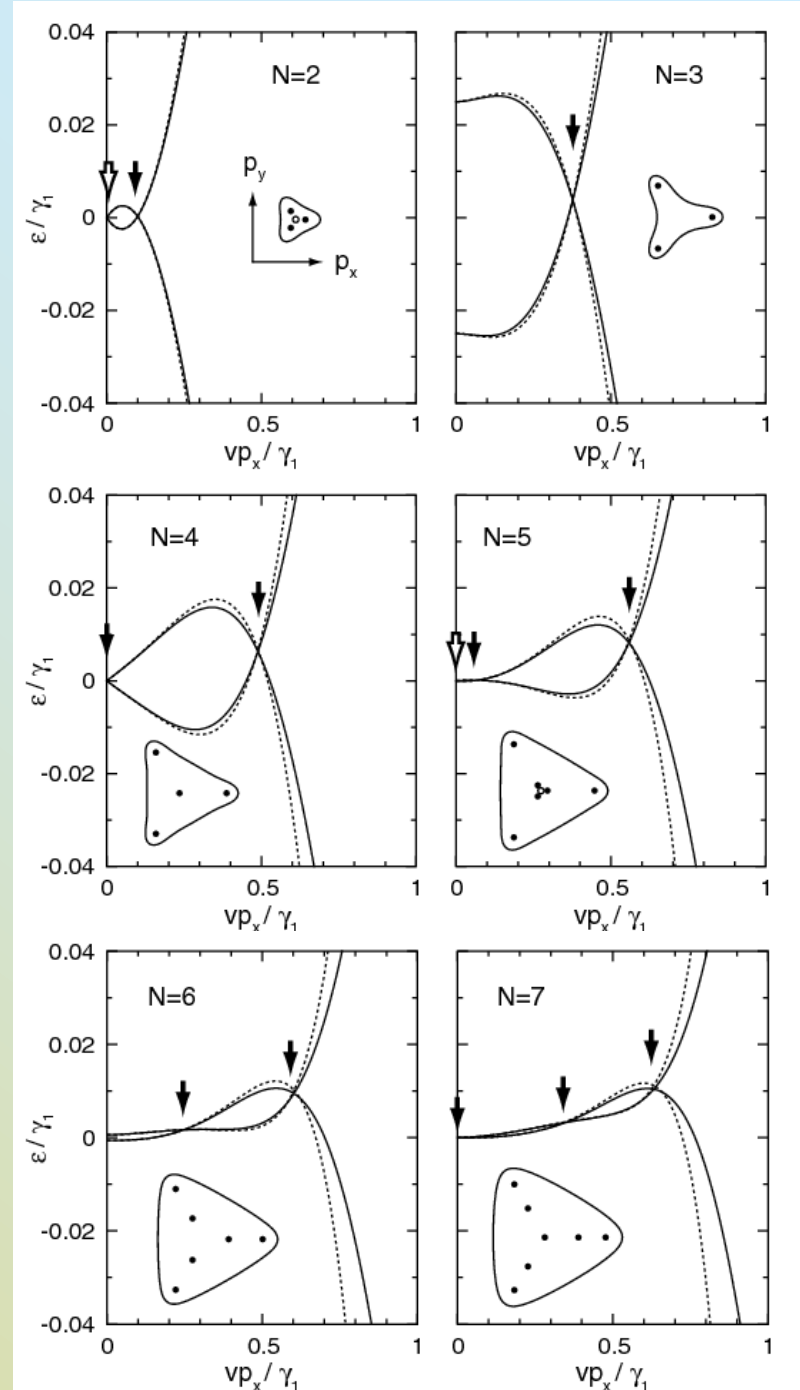


no central pocket

$$\varepsilon_L \approx \frac{\gamma_2}{2} \sim 10 \text{ meV}$$

# Trigonal warping and Berry's phase

for  $N$  layers of  
ABC-stacked multilayers  
(with Berry phase  $N\pi$ )





## AB-stacked bilayer

$$\hat{H}_{bilayer}^{(eff)} =$$

$$-\frac{v^2}{\gamma_1} \begin{pmatrix} 0 & (p_x - ip_y)^2 \\ (p_x + ip_y)^2 & 0 \end{pmatrix} \quad \text{chirality}$$

$$+v_3 \begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix} \quad \text{trigonal warping}$$

$$+\frac{2vv_4 p^2}{\gamma_1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \gamma_4: \text{ e-h asymmetry}$$

$$+\Delta \left[ 1 - \frac{2v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{asymmetry gap}$$

$$+\Delta_{graphite} \left[ 1 - \frac{2v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{more e-h asymmetry}$$

## ABC-stacked trilayer

$$\hat{H}_{ABC}^{(eff)} =$$

$$\frac{v^3}{\gamma_1^2} \begin{pmatrix} 0 & (p_x - ip_y)^3 \\ (p_x + ip_y)^3 & 0 \end{pmatrix}$$

$$+\left[ -\frac{2vv_3 p^2}{\gamma_1} + \frac{\gamma_2}{2} \right] \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$+\frac{2vv_4 p^2}{\gamma_1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$+\Delta_1 \left[ 1 - \frac{v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$+\Delta_2 \left[ 1 - \frac{3v^2 p^2}{\gamma_1^2} \right] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

# Summary

- Trilayers aren't the same as monolayers or bilayers
- ABA-stacked trilayer:
  - Combination of “monolayer” and “bilayer” bands
  - Interlayer asymmetry  $\Delta_1$  hybridises them
  - Two low-energy bands still support chiral quasiparticles
- ABC-stacked trilayer:
  - Cubic generalisation of monolayer and bilayer
  - Lifshitz transition at relatively large energy  $\sim \gamma_2/2 \sim 10\text{meV}$
  - Lifshitz transition into 3 pockets ( $3\pi$ ) not 4 ( $2\pi$ ) as in bilayer.

Mikito Koshino and E. McCann, Physical Review B **79**, 125443 (2009).  
Mikito Koshino and E. McCann, arXiv:0906.4634