

Gapless topological states in bilayer graphene

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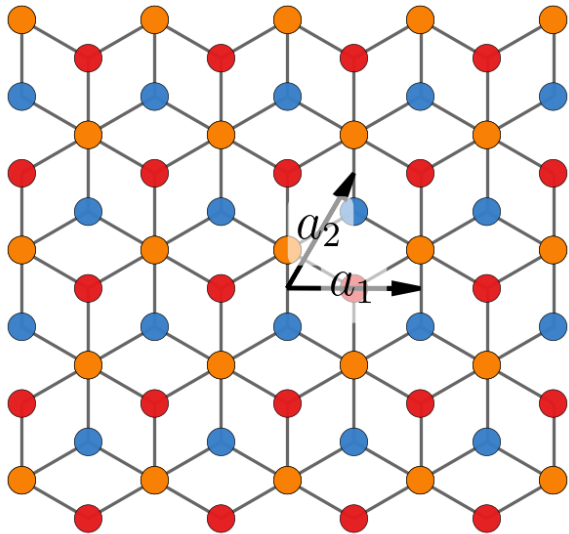
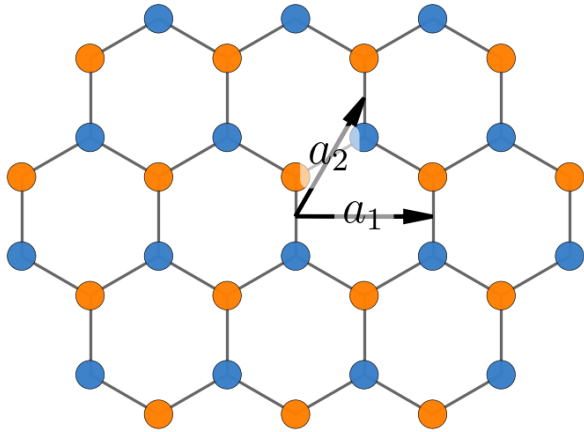
Introduction

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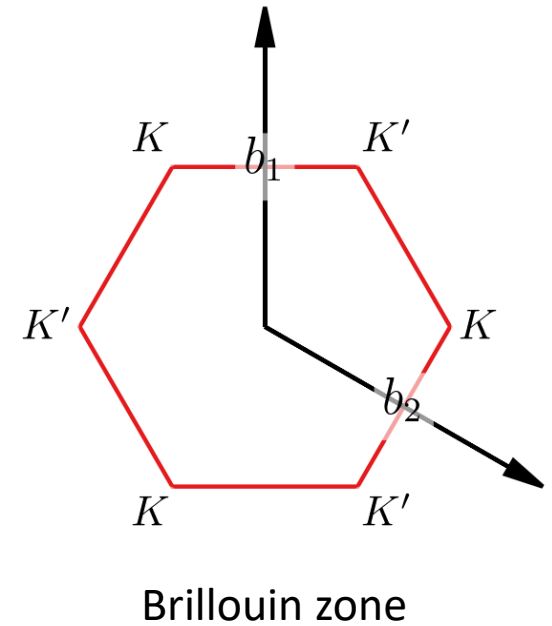
Theoretical description

Defining the system that allow appearance of in-gap states

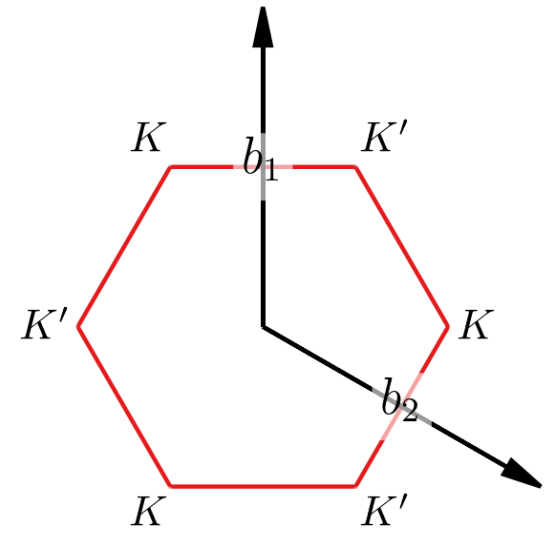
Graphene, monolayer and bilayer



Monolayer and AB stacked bilayer system

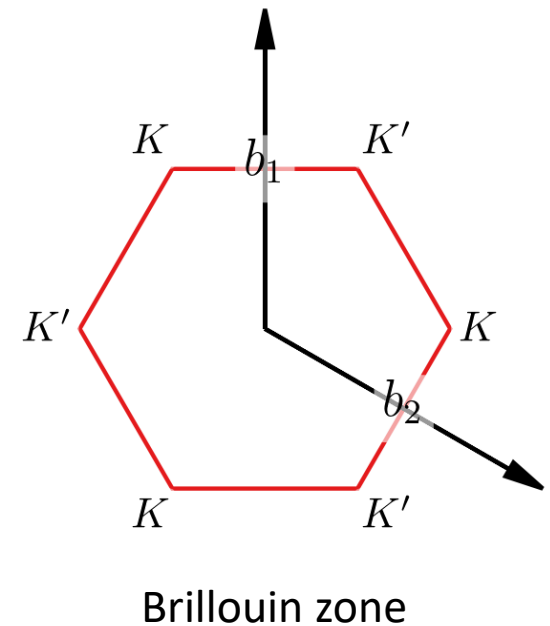
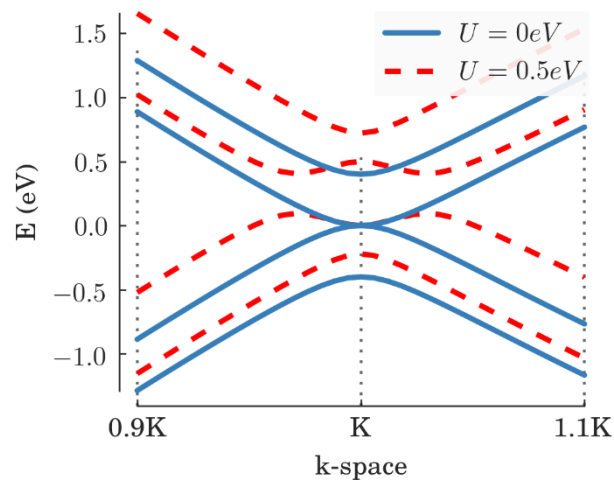
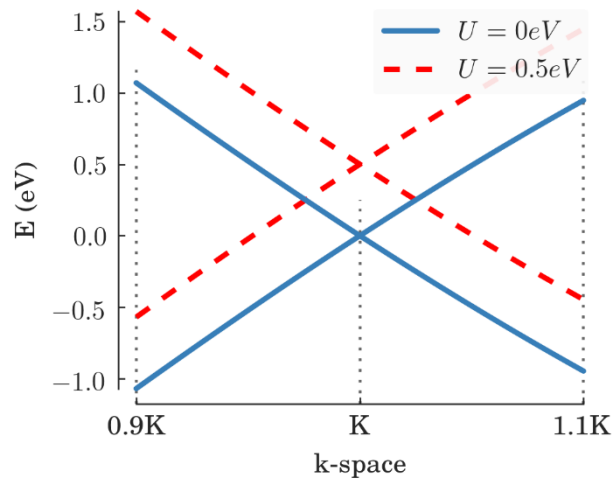


Graphene, monolayer and bilayer



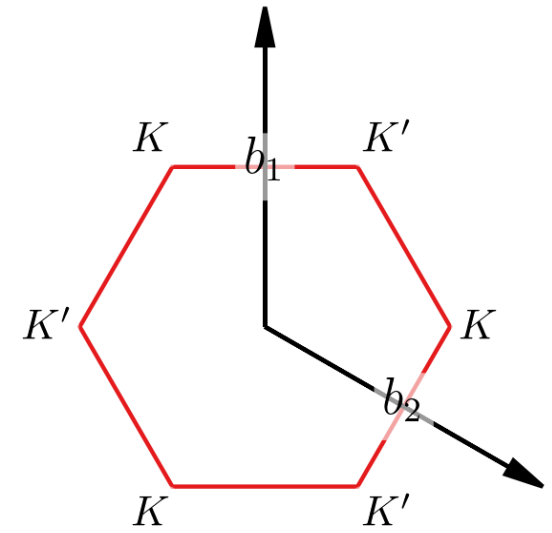
Brillouin zone

Graphene, monolayer and bilayer



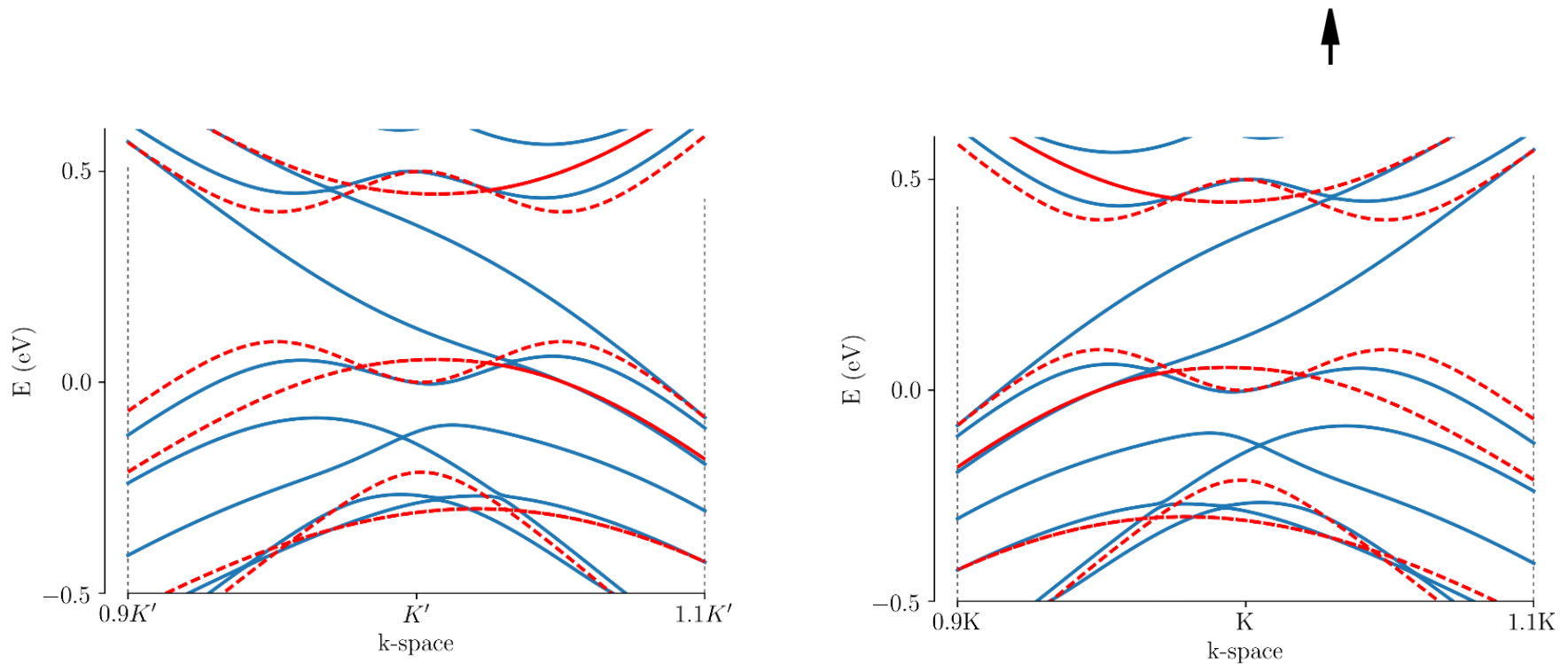
Band structure and electric field effect

Graphene, monolayer and bilayer



Brillouin zone

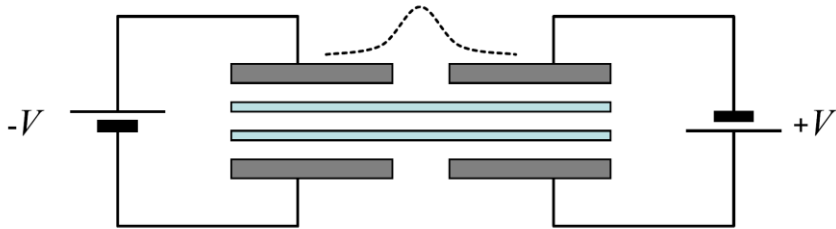
Graphene, monolayer and bilayer



Valley polarized topological states in bilayer graphene AB/BA nanoribbon.

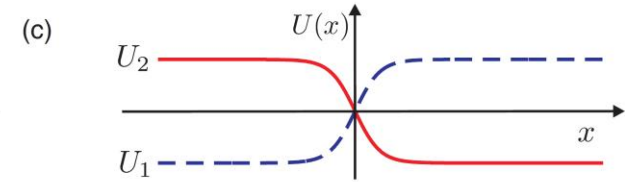
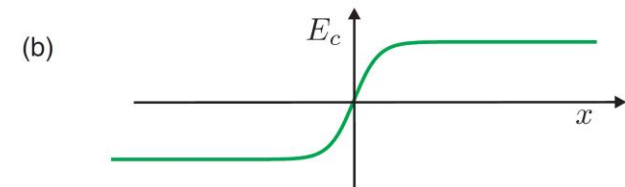
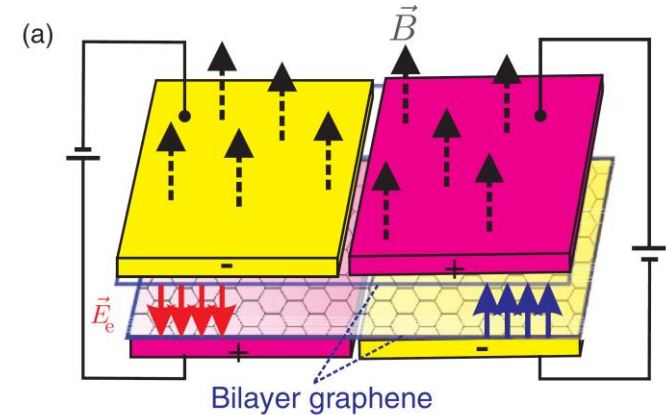
Appearance of in-gap states in bilayer graphene

Kink potential configuration



Martin et al., PRL **100**, 036804 (2008)

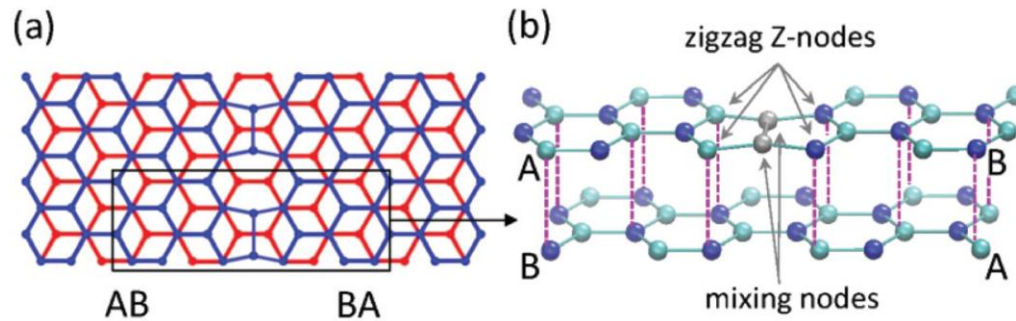
- chiral topological states,
- valley polarized unidirectional motion,
- additional non chiral bands due to kink flattening,
- weakly affected by the magnetic field.



Zarenia et al., PRB **84**, 125451 (2011)

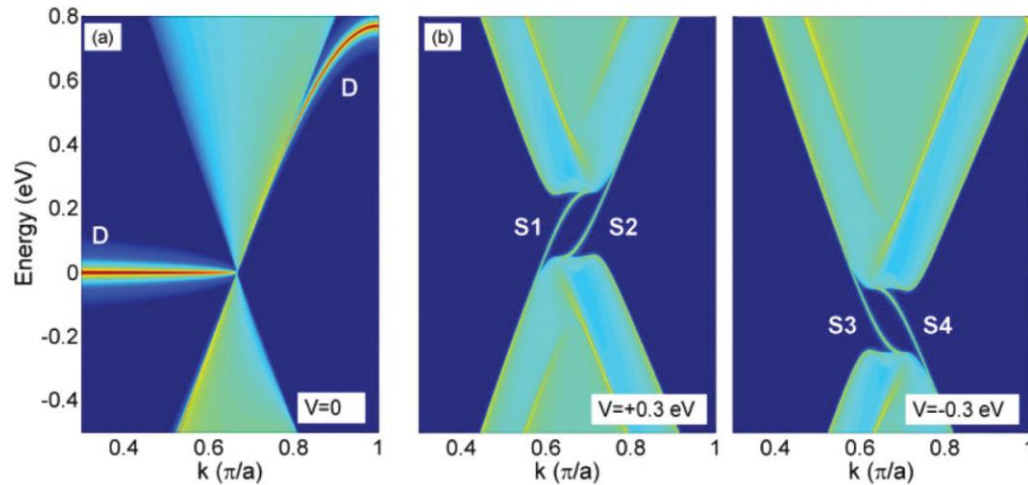
Appearance of in-gap states

Defect line



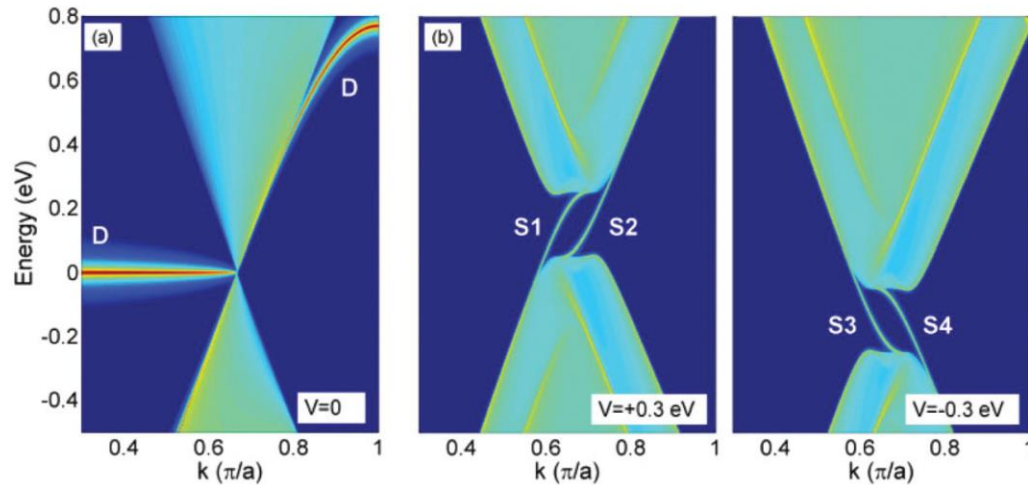
AB/BA stacking bilayer graphene produced by a pentagon-octagon defect line
a) top view, b) bottom view.

Appearance of in-gap states

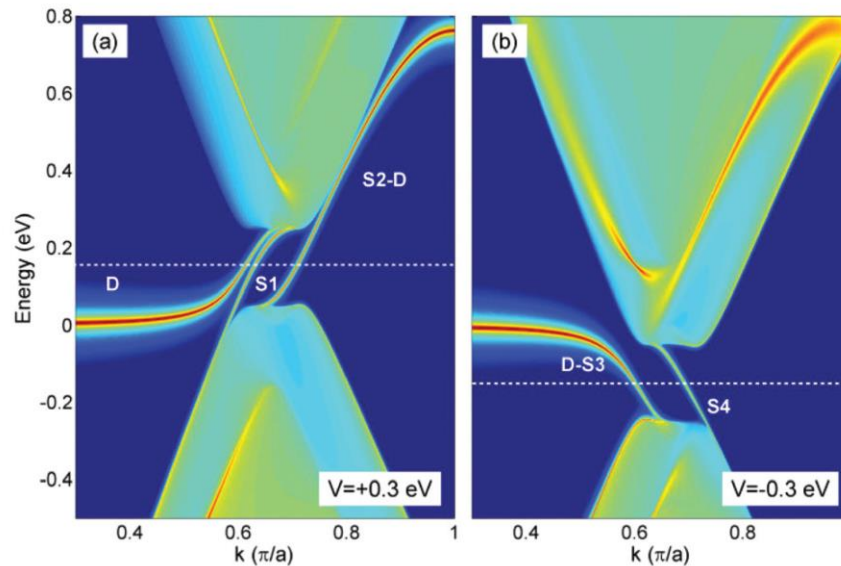


LDOS(k) a) $V=0$ V, with a system with a grain boundary, b), c) AB/BA bilayer graphene (corrugation) with positive and negative voltage applied to the bottom layer.

Appearance of in-gap states



LDOS(k) a) $V=0$ V, with a system with a grain boundary, b), c) AB/BA bilayer graphene (corrugation) with positive and negative voltage applied to the bottom layer.



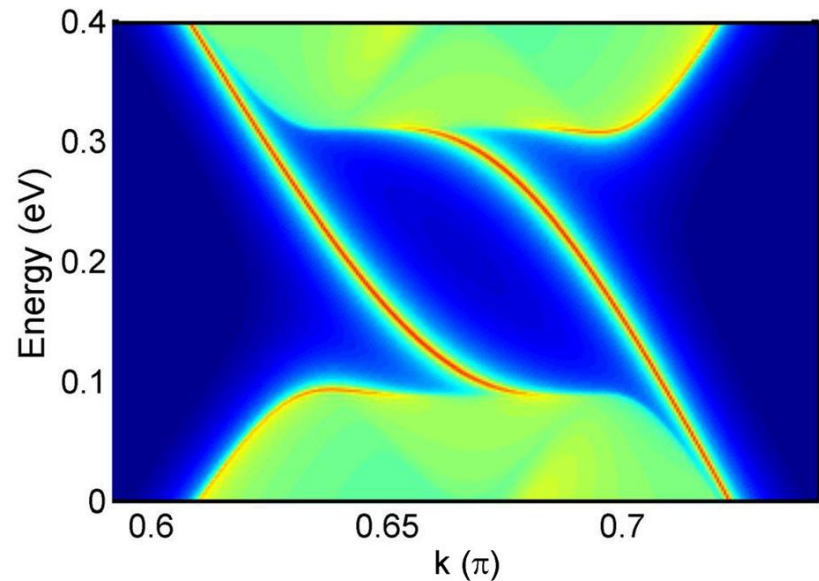
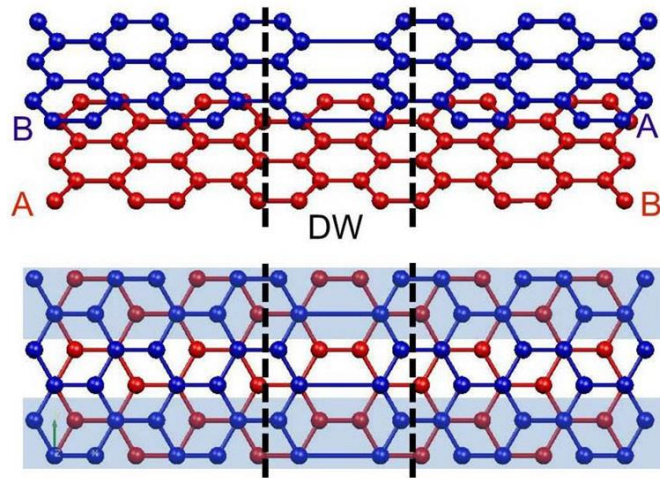
LDOS(k) AB/BA bilayer graphene induced by an octagon-pentagon grain boundary with a) positive and b) negative voltage applied to the bottom layer.

Jaskólski et al., *Nanoscale* **8**, 6079-6084 (2016)

Appearance of in-gap states

Domain wall

Tilt boundary (stacking change) + corrugation (delamination)



- Vaezi *et al.*, PRX **3**, 021918 (2013)
- Zhang *et al.*, PNAS **110**, 10546–10551 (2013)
- Pelc *et al.*, PRB **92**, 085433 (2015)
- Lane *et al.*, PRB **97**, 045301 (2018)
- W Jaskólski *et al.*, 2D Mater. **5** 025006 (2018)

Manipulation

Manipulation

Understanding the motion to be able to design the functionality

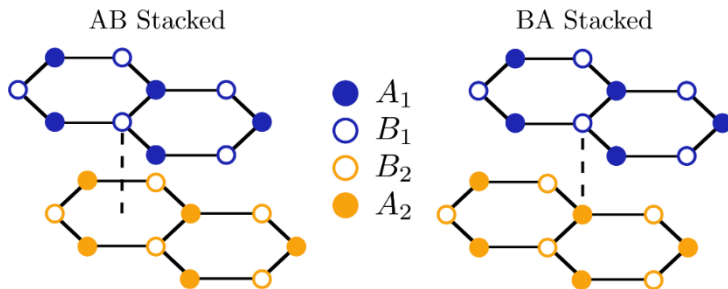
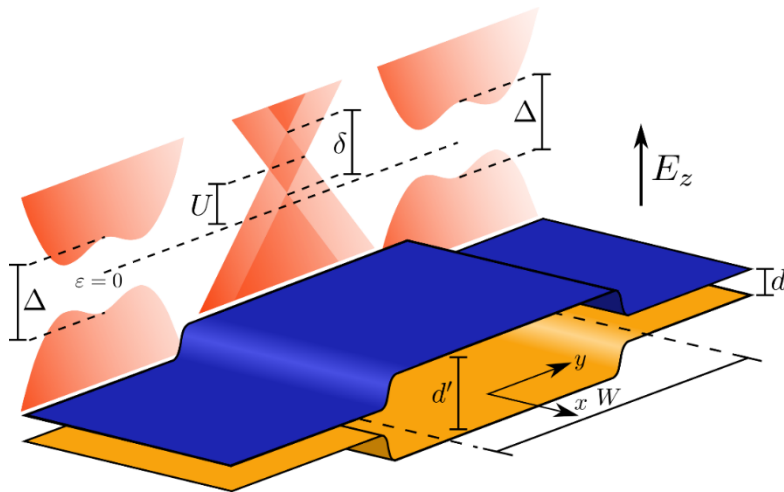
Delamination in bilayer graphene

$$H = - \sum_l \sum_{i,j} \gamma_0 e^{i2\pi\phi_{ij}/\phi_0} c_{l,i}^\dagger c_{l,j} - \sum_{i,j} \{ [(\theta(y_i) + (\theta(y_i - W)))] \gamma_1 c_{1,i}^\dagger c_{2,j} + H.C. \} + \sum_i V_\pm c_i^\dagger c_i$$

$$\gamma_0 = 3.1 \text{ eV}$$

$$\gamma_1 = 0.39 \text{ eV}$$

$$V_\pm = \Delta(y_i) + U(y_i) + \delta(y_i)$$



Lane *et al.*, PRB **97**, 045301 (2018)

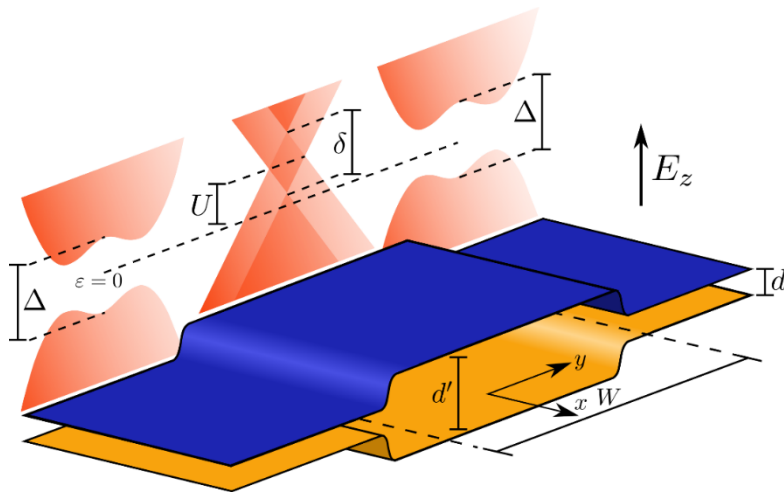
Delamination in bilayer graphene

$$H = - \sum_l \sum_{i,j} \gamma_0 e^{i2\pi\phi_{ij}/\phi_0} c_{l,i}^\dagger c_{l,j} - \sum_{i,j} \{ [(\theta(y_i) + (\theta(y_i - W)))] \gamma_1 c_{1,i}^\dagger c_{2,j} + H.C. \} + \sum_i V_\pm c_i^\dagger c_i$$

$$\gamma_0 = 3.1 \text{ eV}$$

$$\gamma_1 = 0.39 \text{ eV}$$

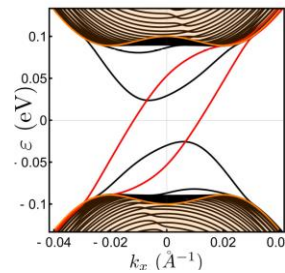
$$V_\pm = \Delta(y_i) + U(y_i) + \delta(y_i)$$



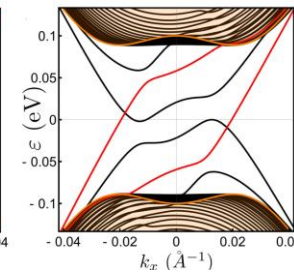
$$U = 0 \text{ eV}$$

$$\Delta = 0.2 \text{ eV}$$

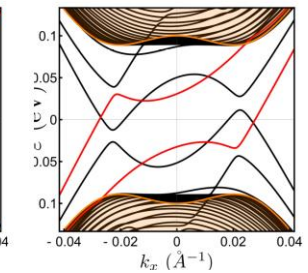
$$\delta = 0.2 \text{ eV}$$



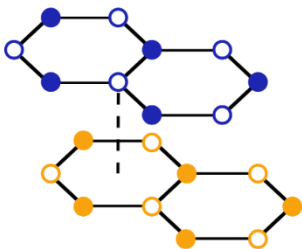
$$\delta = 0.3 \text{ eV}$$



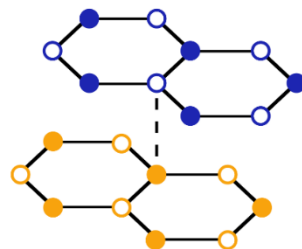
$$\delta = 0.4 \text{ eV}$$



AB Stacked



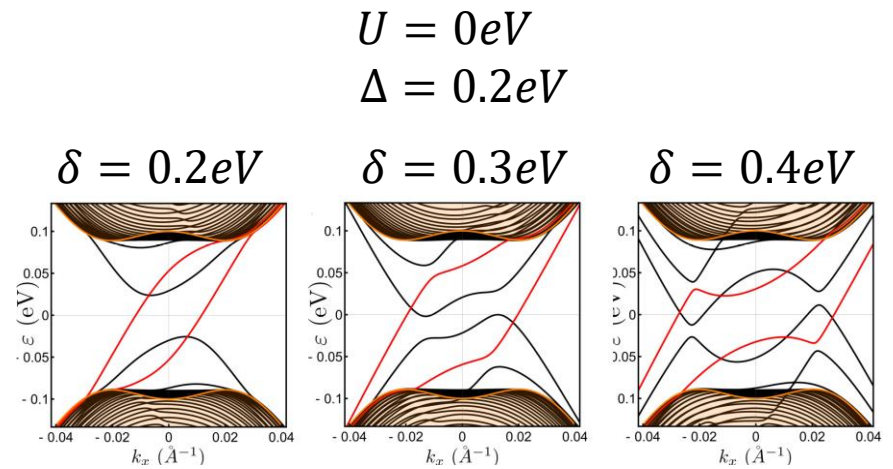
BA Stacked



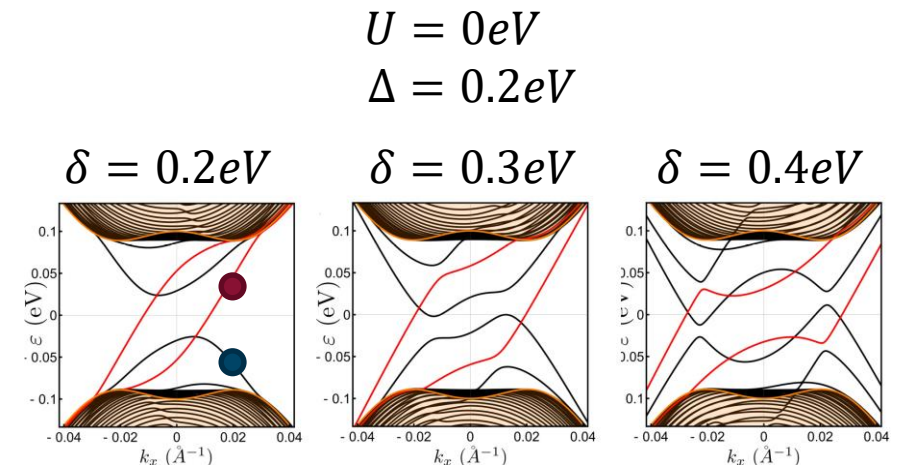
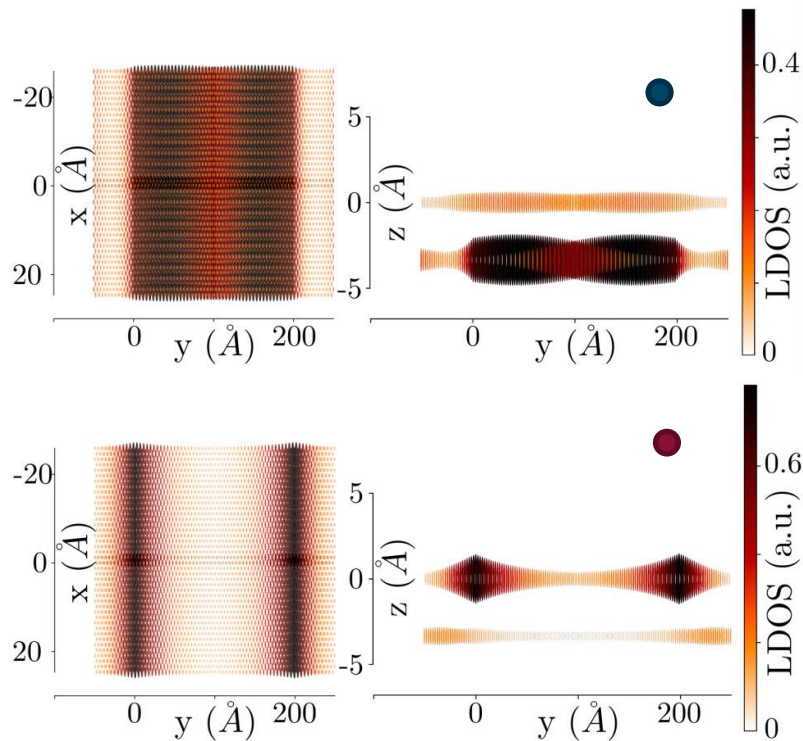
- A_1
- B_1
- B_2
- A_2

Lane *et al.*, PRB **97**, 045301 (2018)

Delamination in bilayer graphene



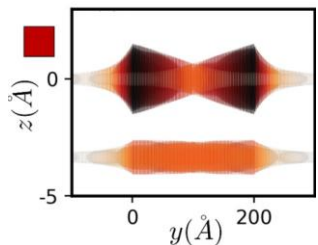
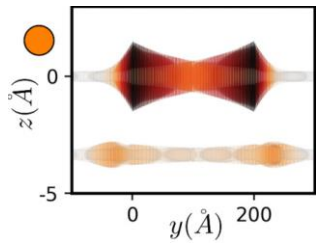
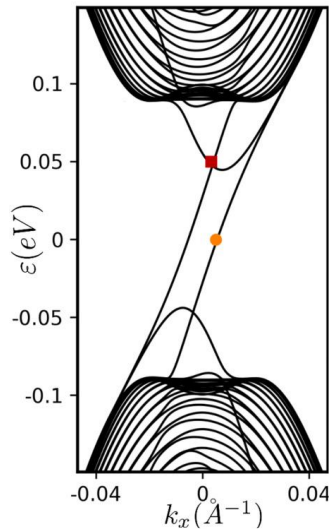
Delamination in bilayer graphene



- localized along the edges,
- monolayer bouncing bands are distributed along delamination.

Delamination in magnetic field

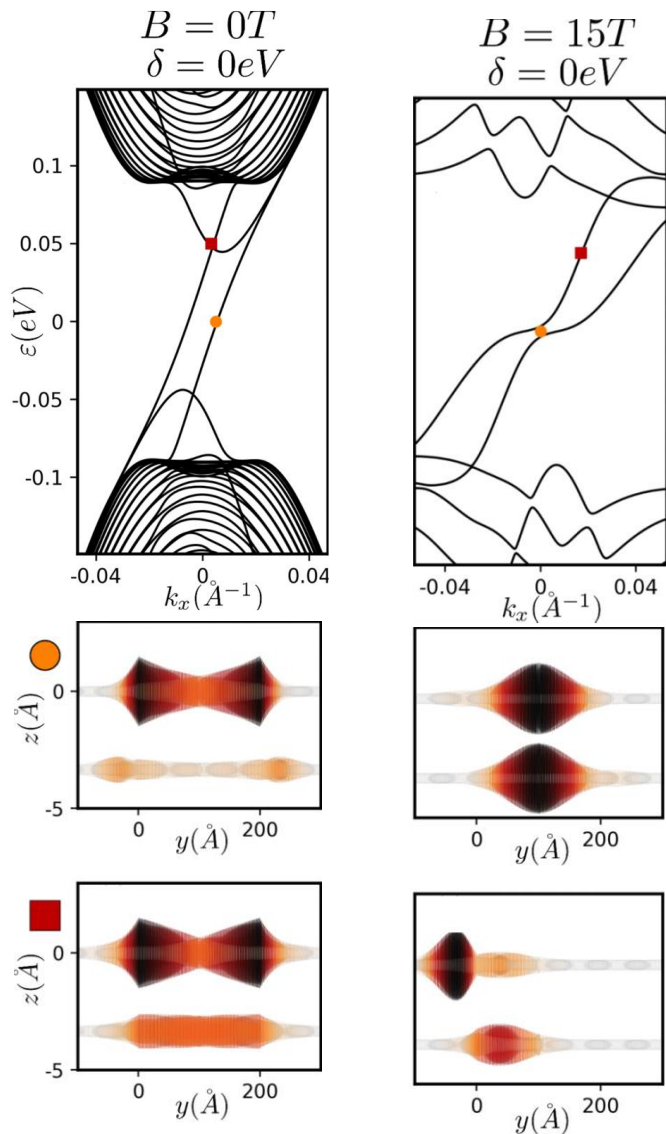
$$B = 0T$$
$$\delta = 0eV$$



$$r_0 \sim l_B = \sqrt{\hbar/eB} < W/2$$

$$\vec{F}_L = e\vec{v} \times \vec{B}$$

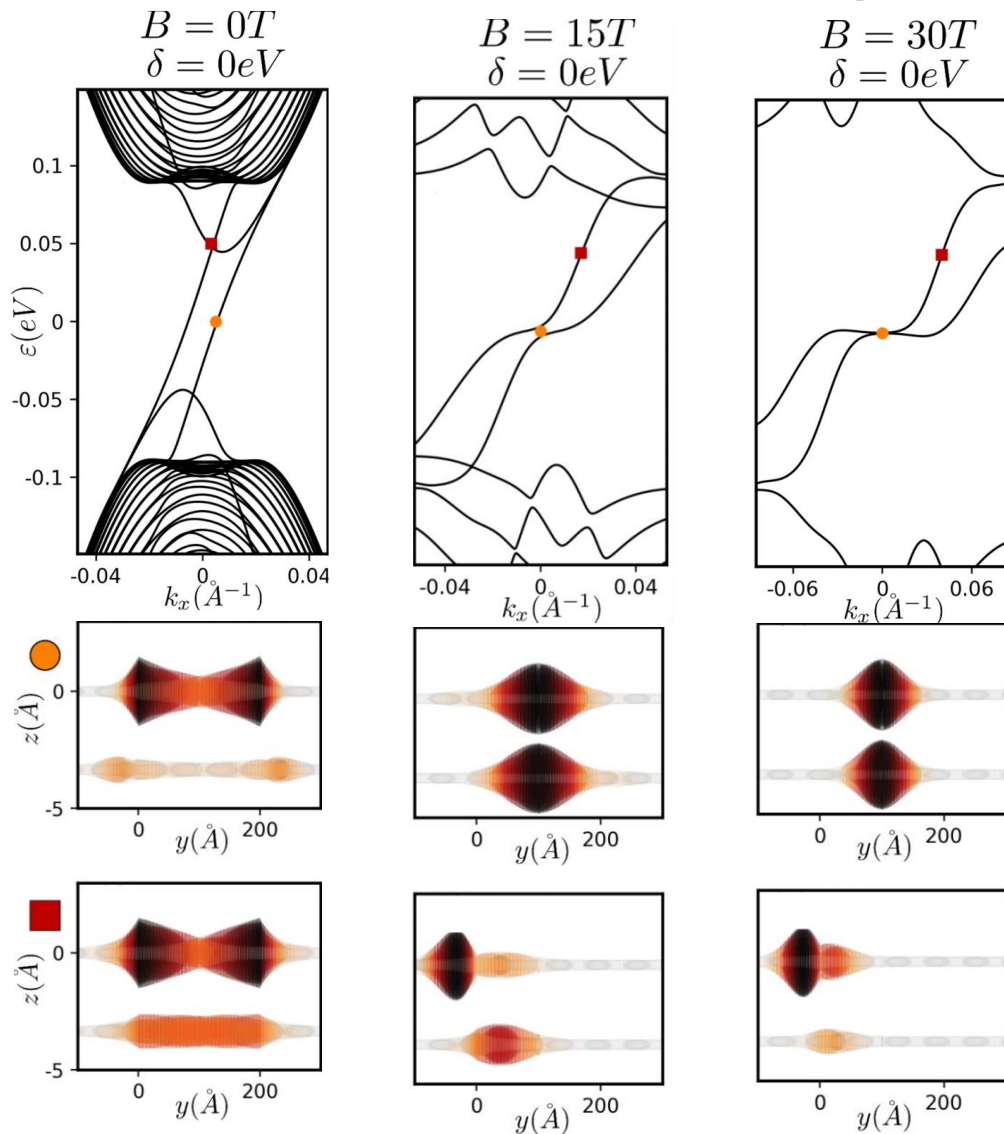
Delamination in magnetic field



$$r_0 \sim l_B = \sqrt{\hbar/eB} < W/2$$

$$\vec{F}_L = e\vec{v} \times \vec{B}$$

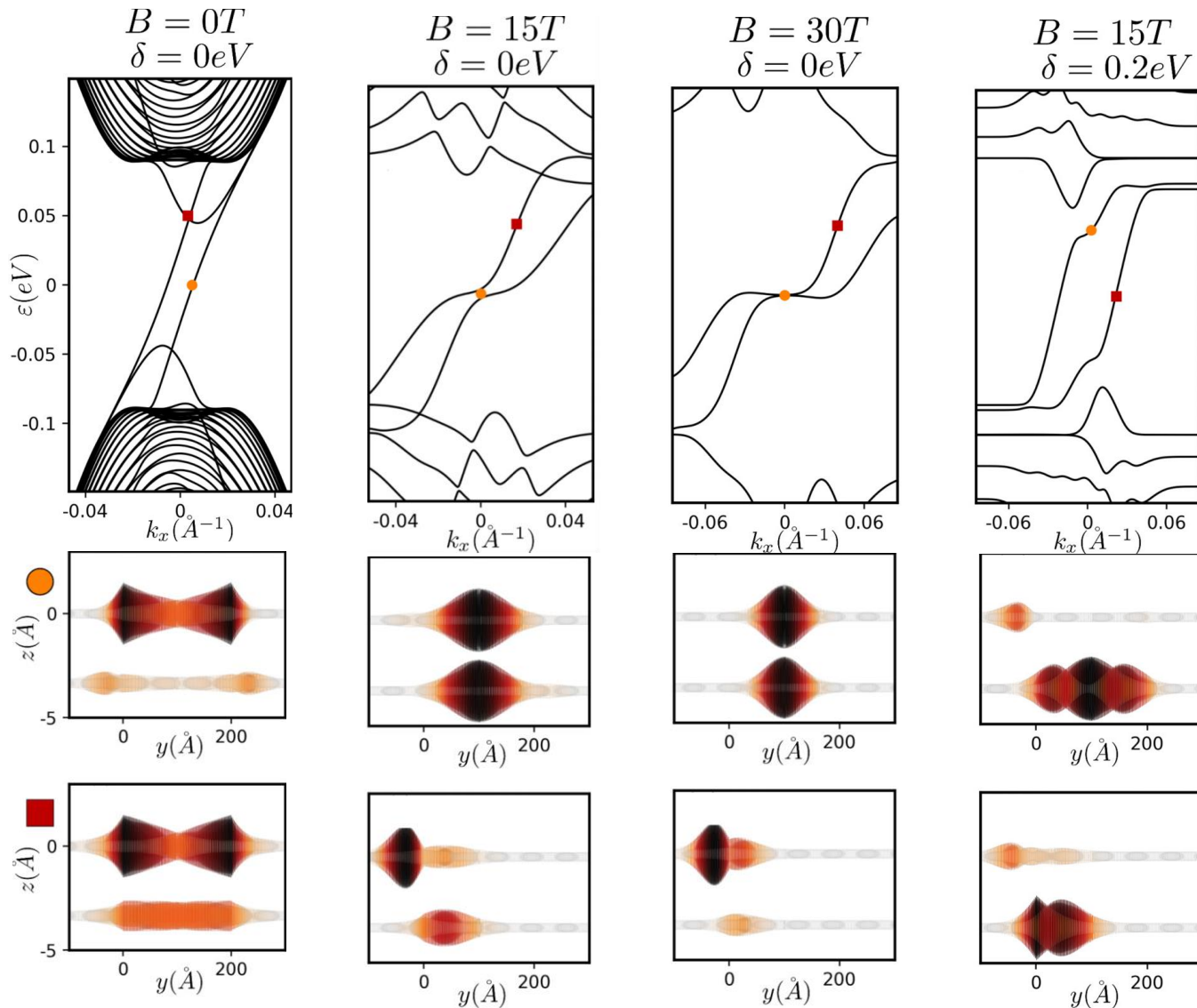
Delamination in magnetic field



$$r_0 \sim l_B = \sqrt{\hbar/eB} < W/2$$

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Delamination in magnetic field



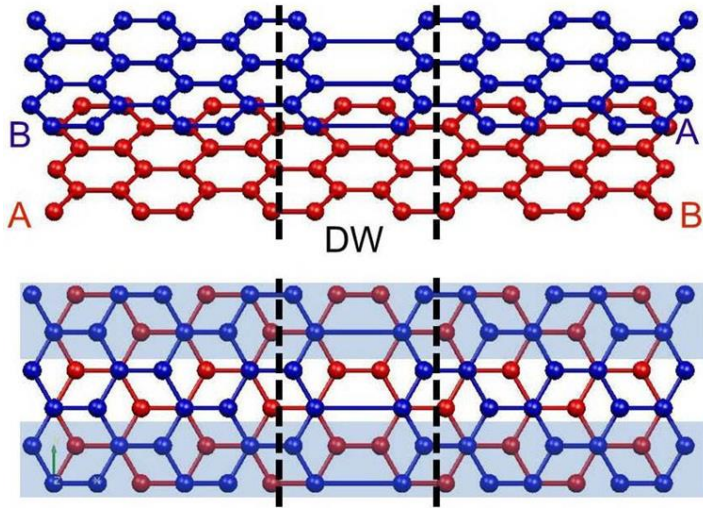
$$r_0 \sim l_B = \sqrt{\hbar/eB} < W/2$$

$$\vec{F}_L = e\vec{v} \times \vec{B}$$

$-\vec{F}_L$ is acting on the modes
 - monolayer bands are forming LL.

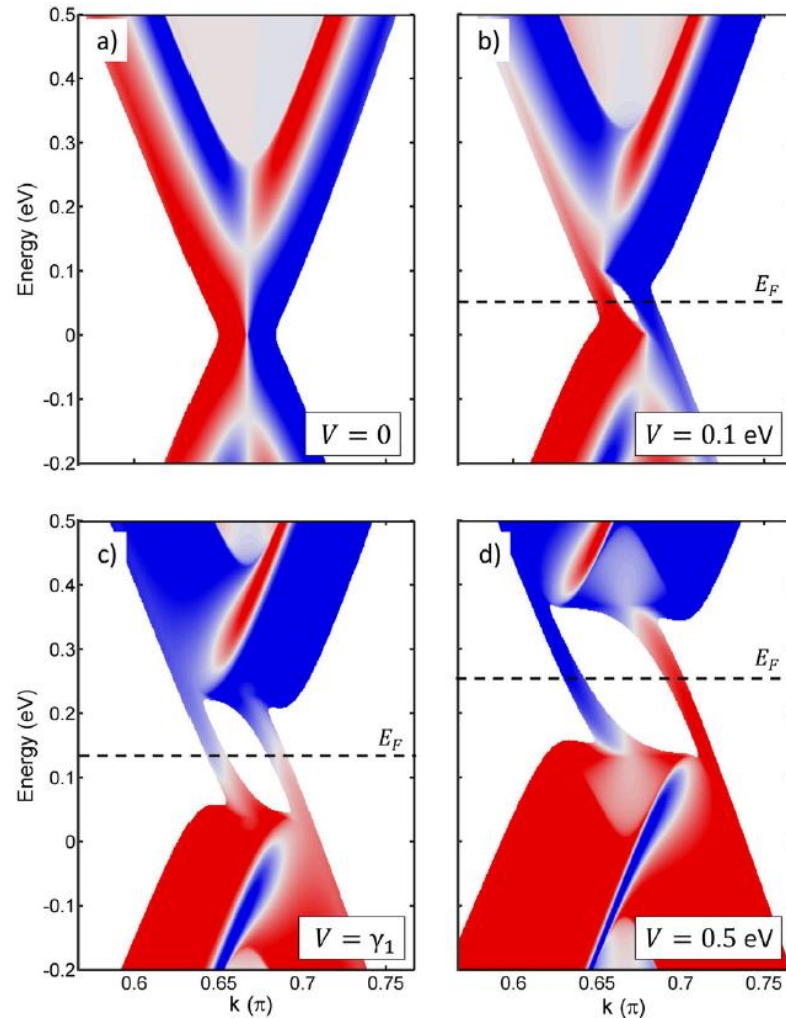


Layer polarization



AB/domain wall/BA nanoribbon

- layer degree of freedom beside the valley and sublattice,
- tuned by doping and modified by electric field.



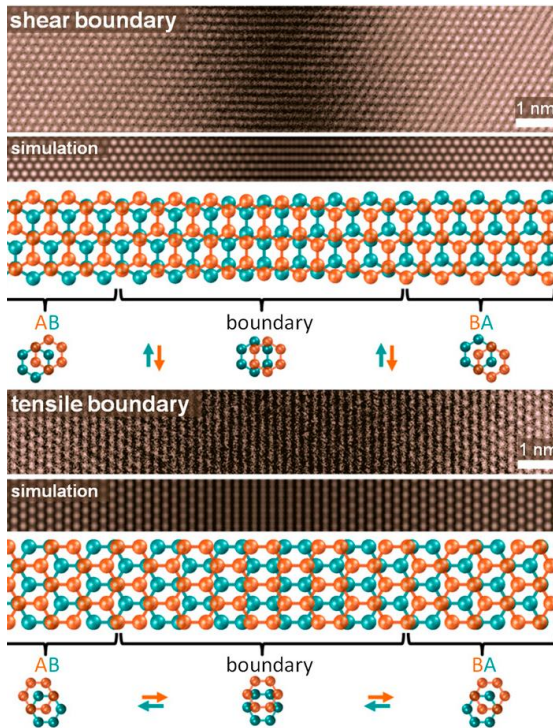
Layer dependent LDOS(k). Red and blue show localization in top and bottom layer respectively

Gapless states in gated bilayer. Is the gated bilayer really gapped?

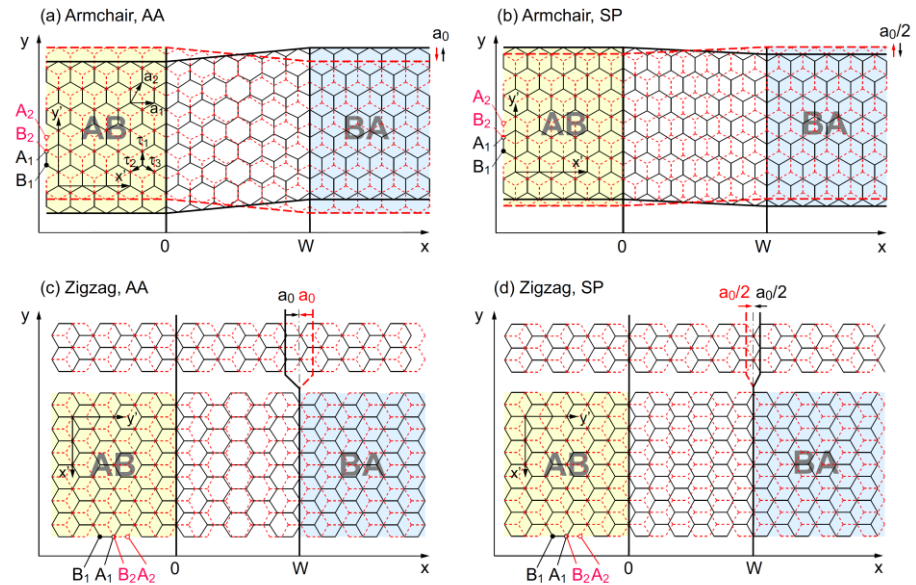
Oostinga *et al.*, Nature Materials **7**, 151–157 (2008) ~ bellow 50 meV

Zhang *et al.*, Nature (London) **459**, 820–823 (2009) ~ 250 meV

Domain walls, stacking solitons



Obtaining different stacking through domain wall, strain soliton

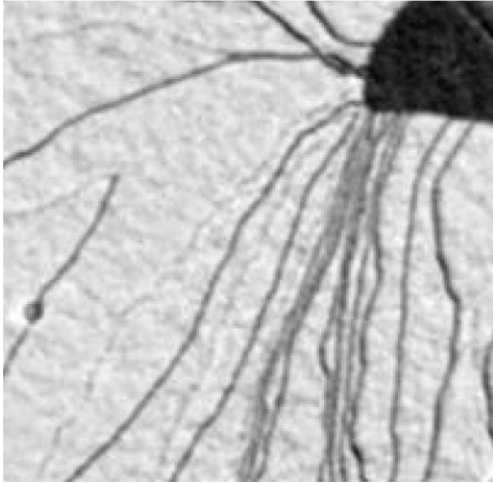


STEM images and simulation of AB-BA domain boundary, shear + tensile strain soliton.

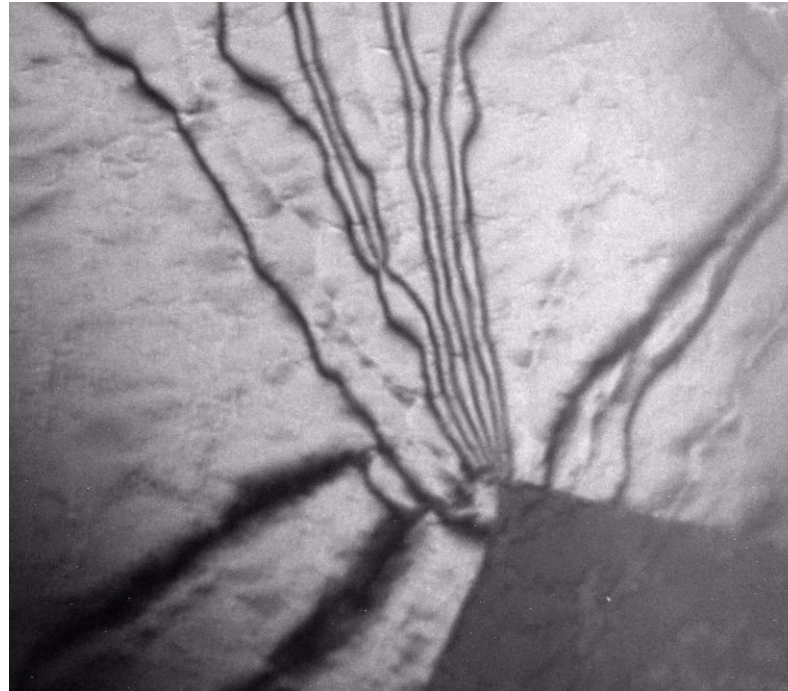
Koshino, PRB **11**, 115409 (2013)

Alden *et al.*, PNAS **110** (28), 11256-11260 (2013)

Change of stacking

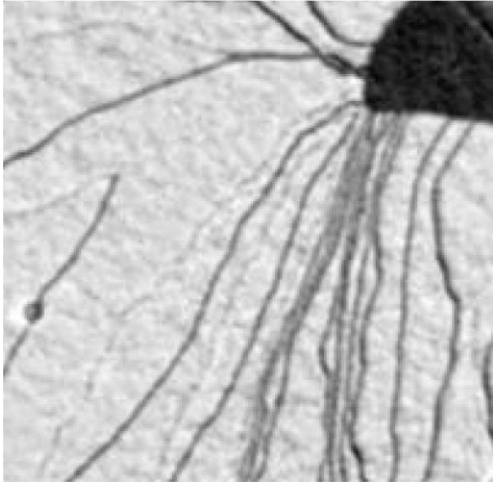


Dark-field TEM of a large bilayer graphene flake.



Lin *et al.*, *Nano Lett.* **13** (7),
3262–3268 (2013)

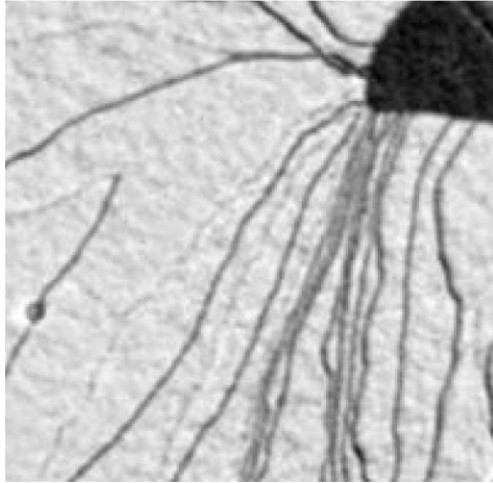
Change of stacking



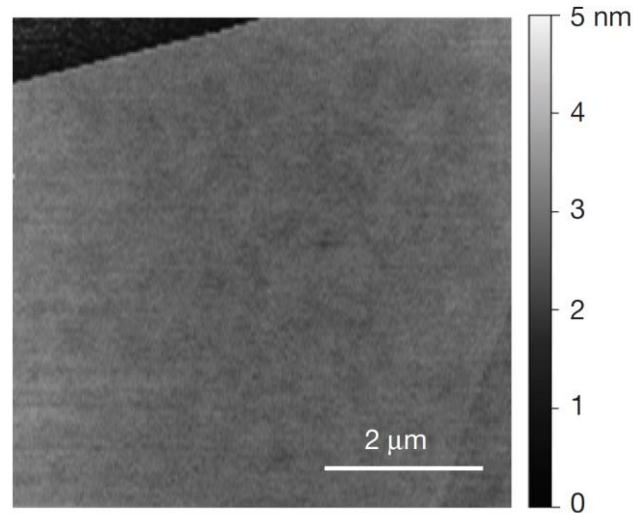
Dark-field TEM of a
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graphene flake.

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3262–3268 (2013)

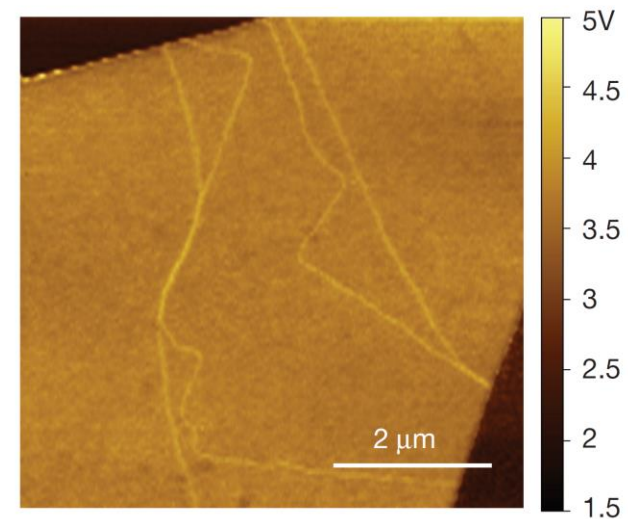
Change of stacking



Dark-field TEM of a large bilayer graphene flake.



AFM topography map of bilayer graphene on SiO₂/Si + graphene monolayer bottom right.



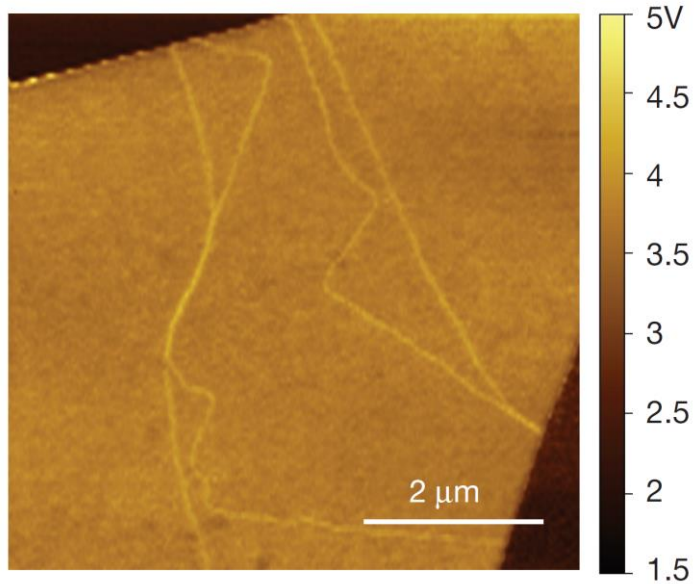
Near-field infrared nanoscopy of the same sample.

Lin *et al.*, Nano Lett. **13** (7), 3262–3268 (2013)

Ju *et al.*, Nature **520** (7549), 650–655 (2015)

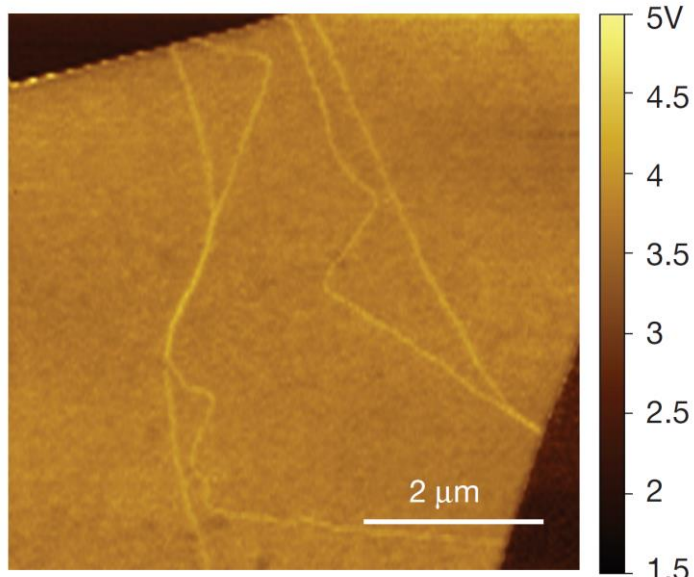
Experimental observation and realization possibilities

Topological transport at a domain wall

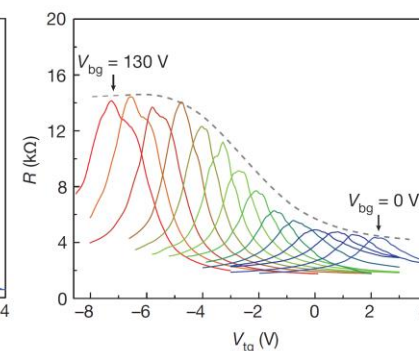
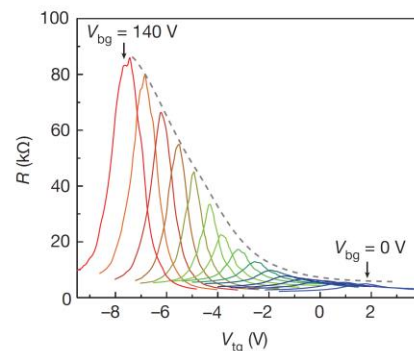
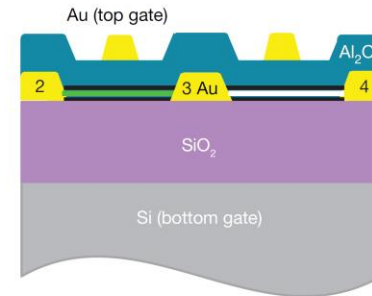
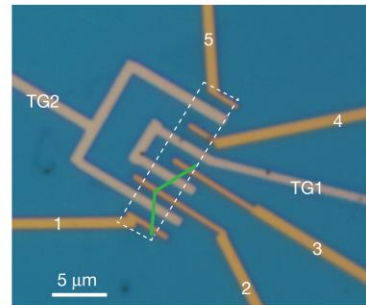


AB/BA domain walls in
exfoliated bilayer graphene

Topological transport at a domain wall



AB/BA domain walls in exfoliated bilayer graphene

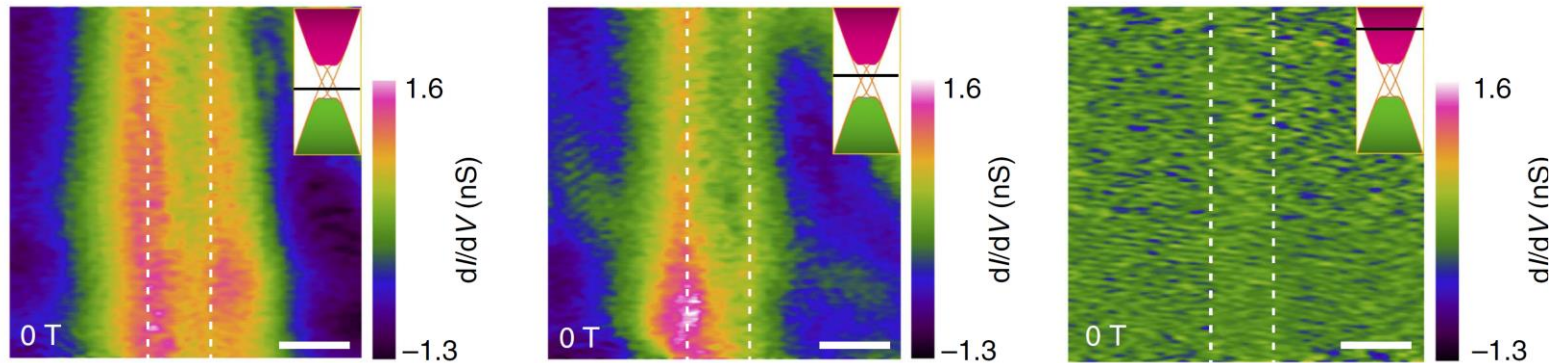


Gating a bilayer graphene flake, sample with and without a domain wall. Applied perpendicular electric field, appearance of boundary states.

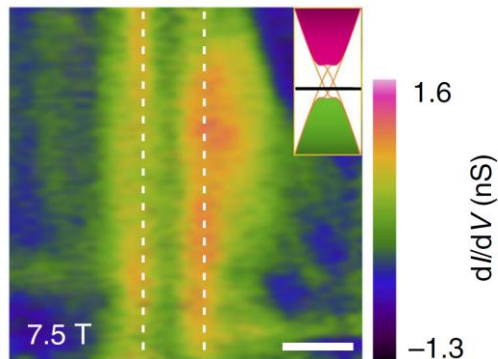
- conductance on the order of $\frac{2e^2}{h}$, smaller due to gate resistance, shorter channels up to $\frac{4e^2}{h}$
- MFP up to 400 nm,
- limitation random appearance.

Ju *et al.*, *Nature* **520**, 650–655 (2015)

Imaging of topological states



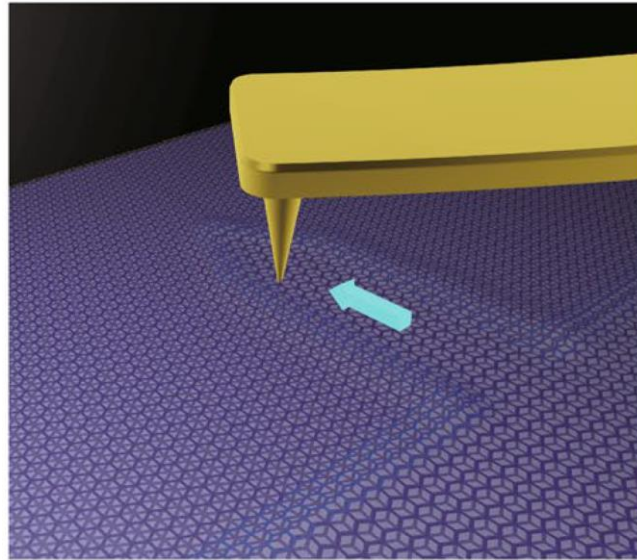
STM image of the domain wall states. Dependence on the Fermi energy.



Imaging the domain wall states in the magnetic field.

Manipulation of domain walls

- move, erase, and split the domain walls with an AFM tip,
- most are stable at room temperature.



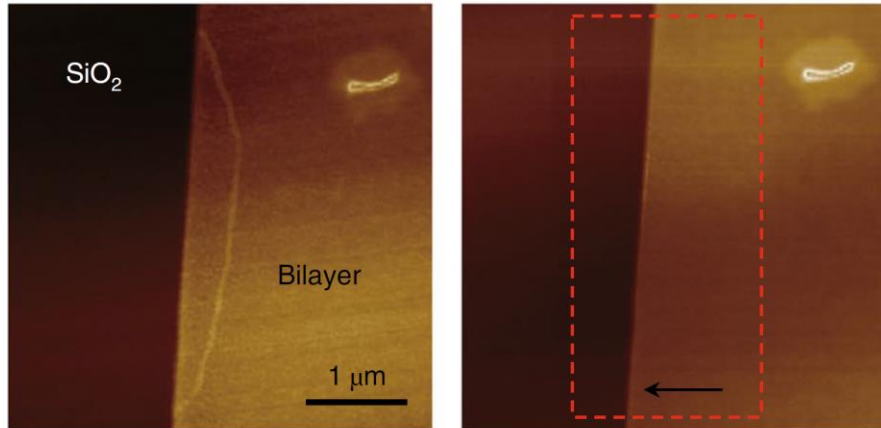
Manipulation of domain walls

Jiang *et al.*, *Nat. Nano. Letters* (2018)



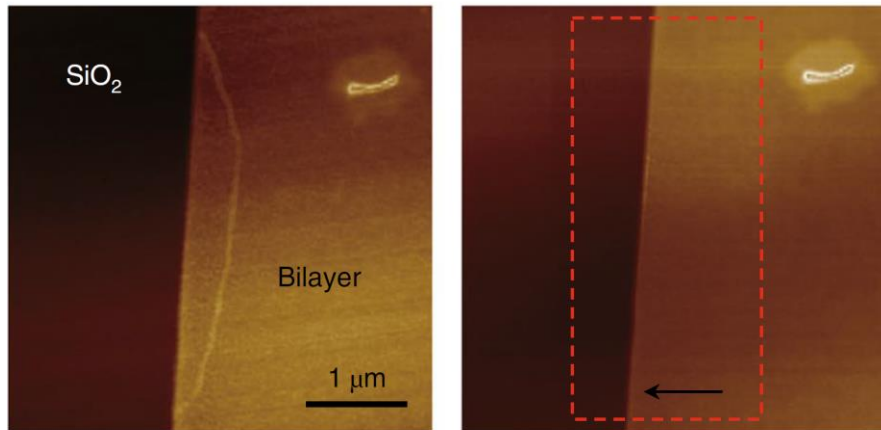
Manipulation of domain walls

Erasing

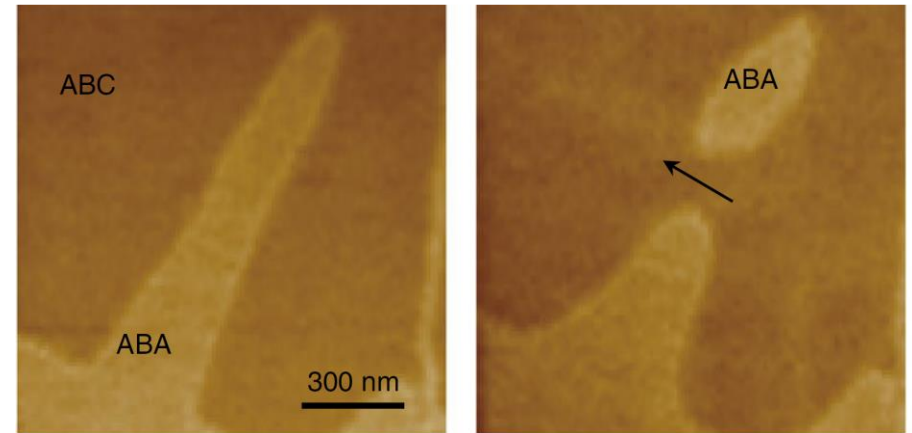


Manipulation of domain walls

Erasing

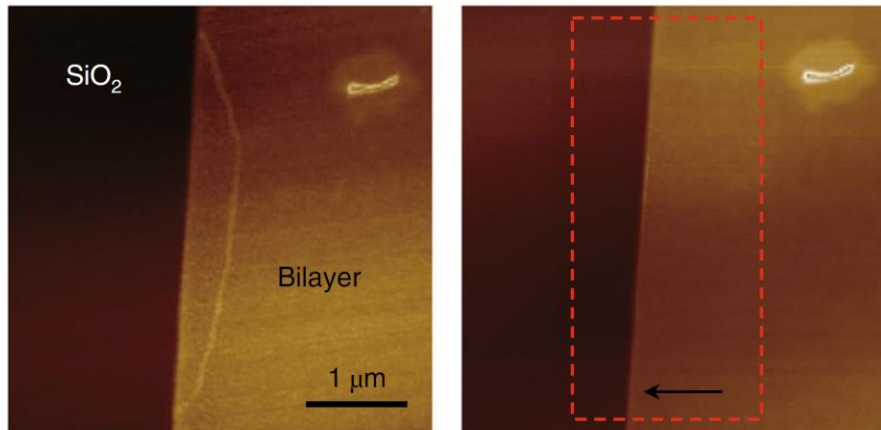


Splitting

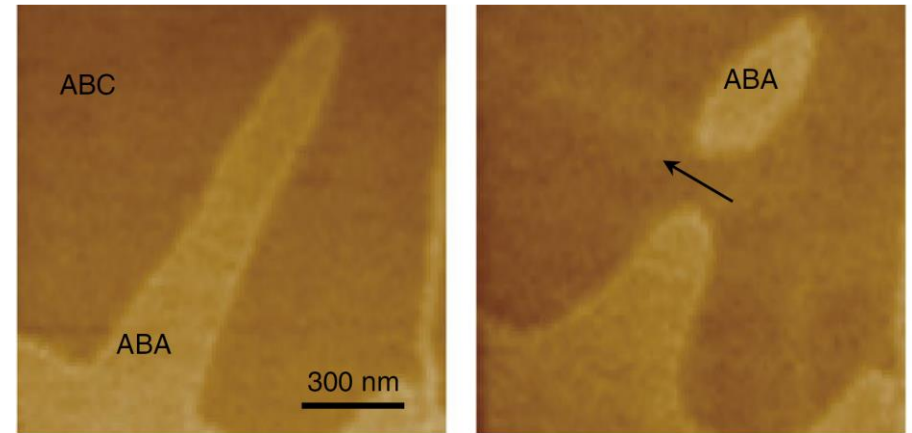


Manipulation of domain walls

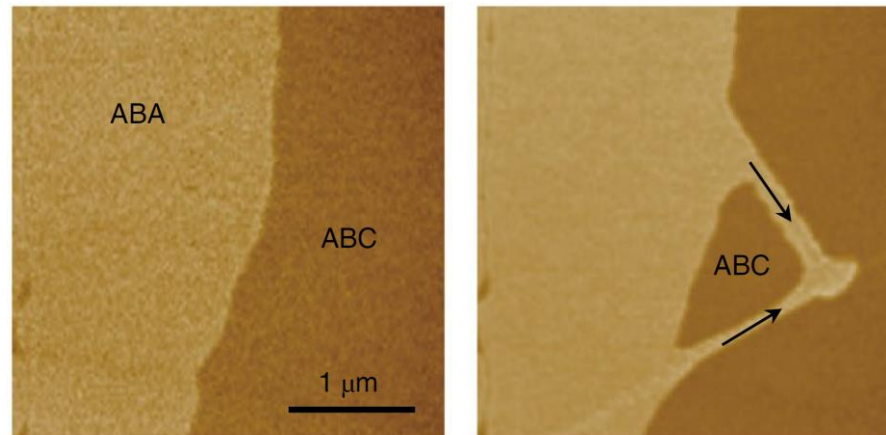
Erasing



Splitting



Moving

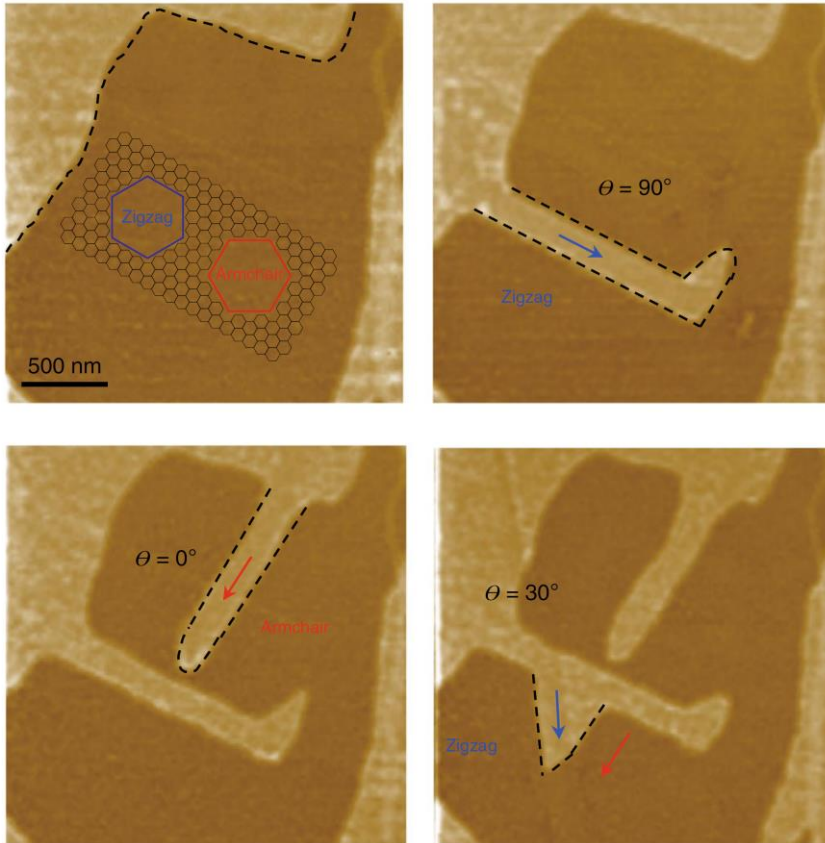


Near-field infrared nanoscopy images of treated samples of bilayer and trilayer graphene

Jiang *et al.*, *Nat. Nano. Letters* (2018)

Manipulation of domain walls

Anisotropy in creation

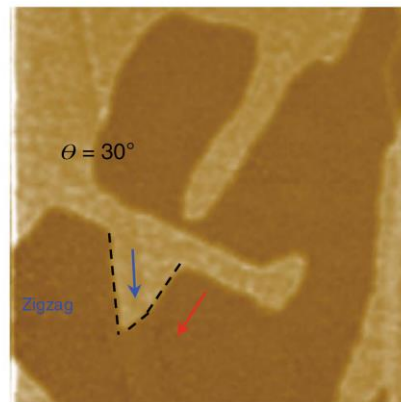
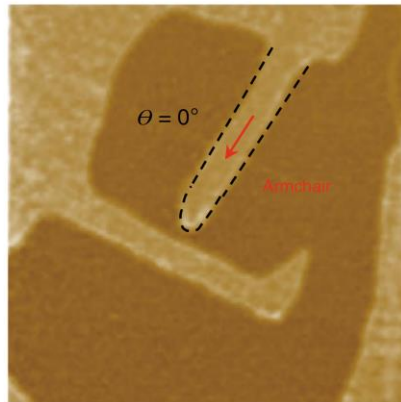
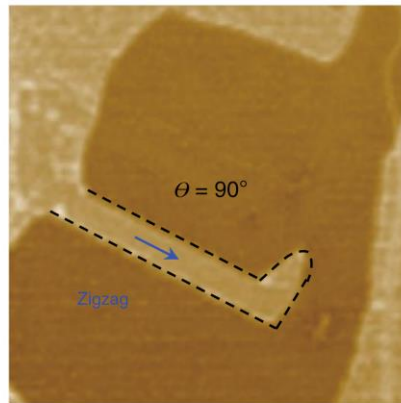
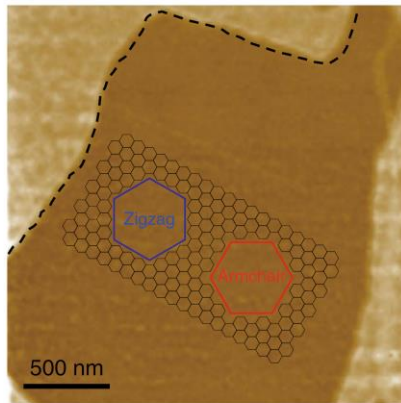


Creation of different shapes

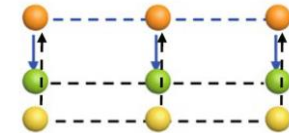
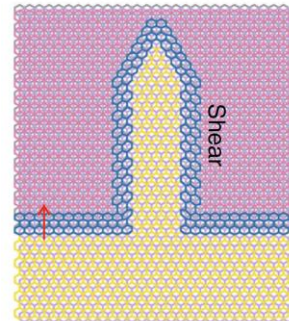
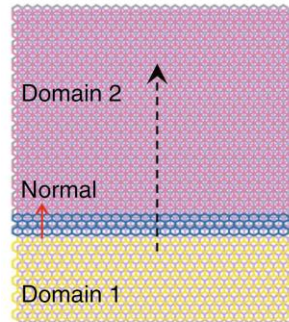
Jiang *et al.*, *Nat. Nano. Letters* (2018)

Manipulation of domain walls

Anisotropy in creation



rounded
rectangular



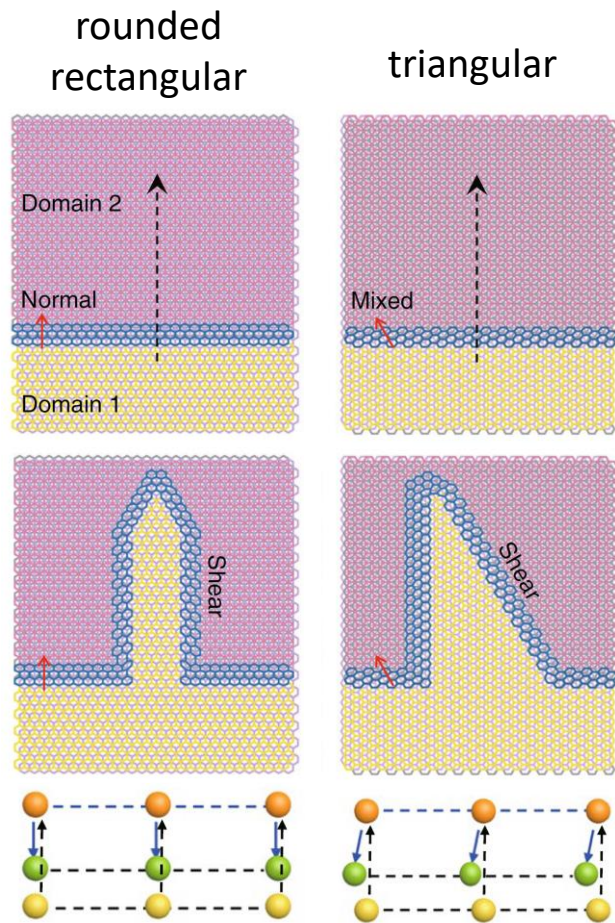
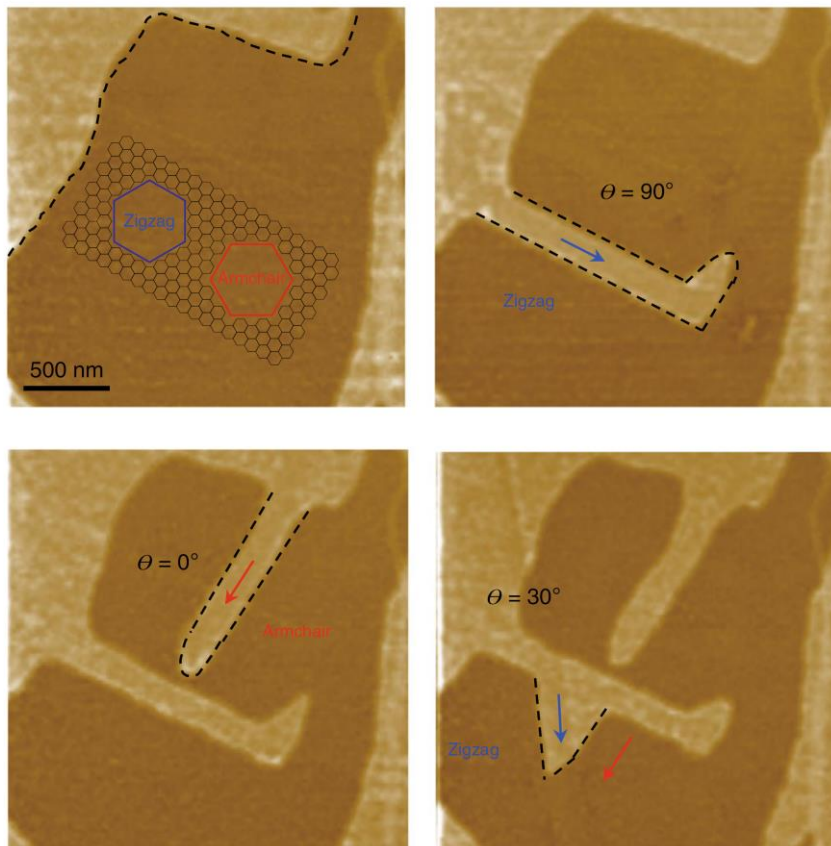
Creation of different shapes

- Initial site
- Non-equilibrium site
- Bernal or rhombohedral stacking site

Jiang *et al.*, *Nat. Nano. Letters* (2018)

Manipulation of domain walls

Anisotropy in creation



Creation of different shapes

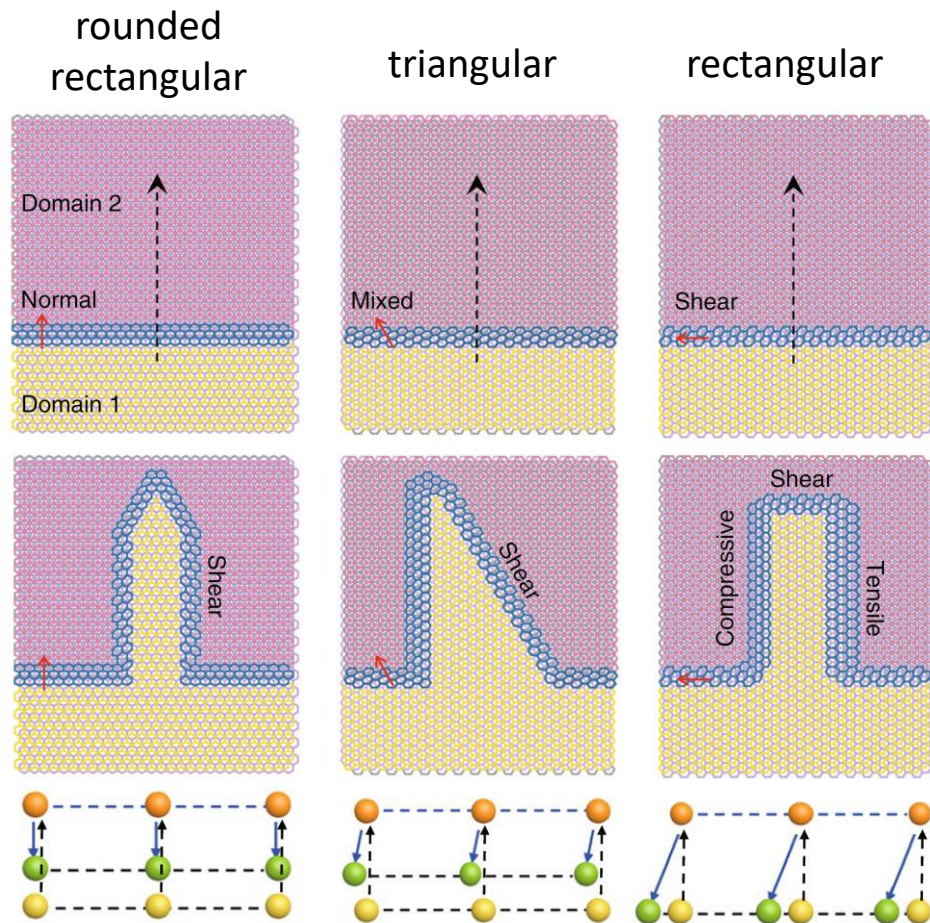
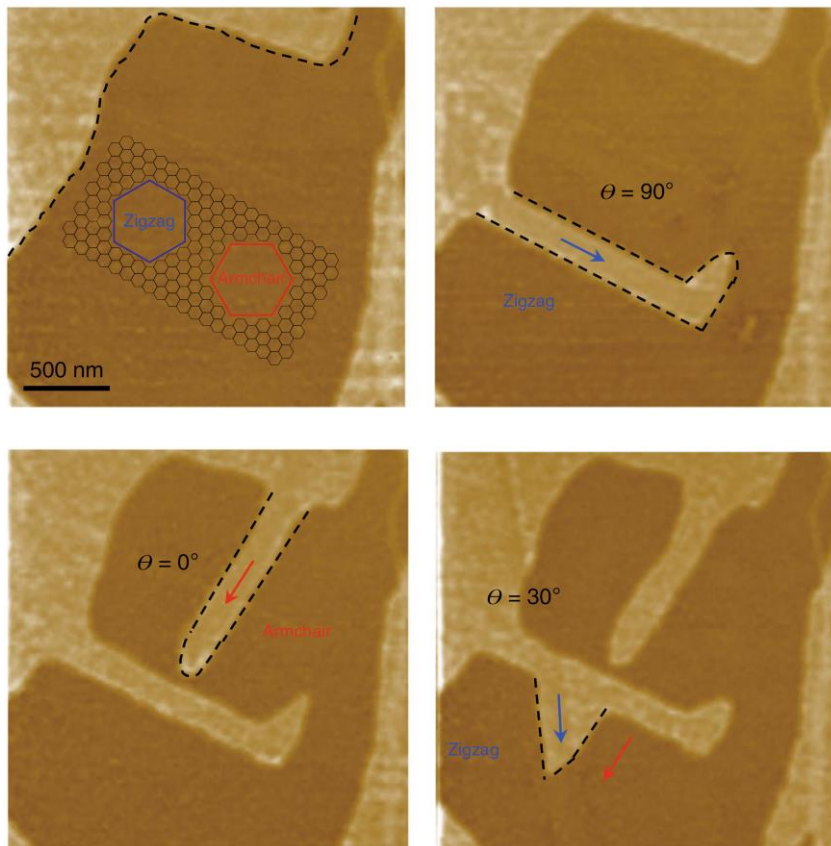
- Initial site
- Non-equilibrium site
- Bernal or rhombohedral stacking site

Jiang *et al.*, *Nat. Nano. Letters* (2018)



Manipulation of domain walls

Anisotropy in creation



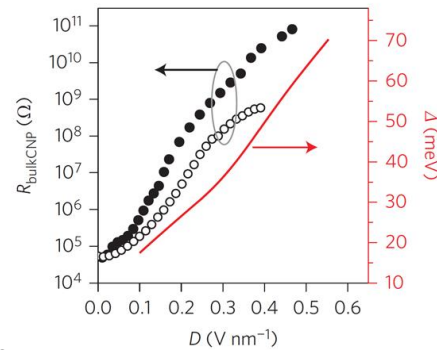
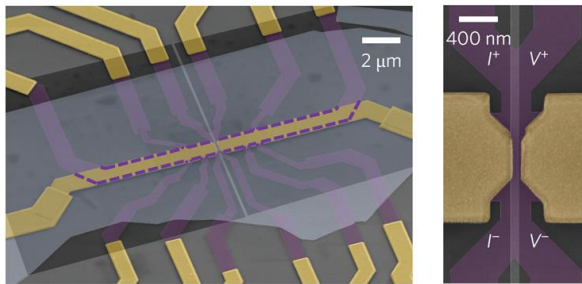
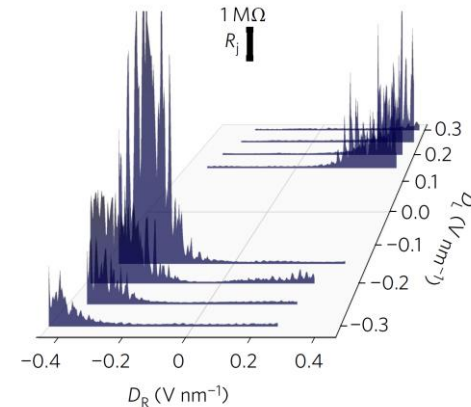
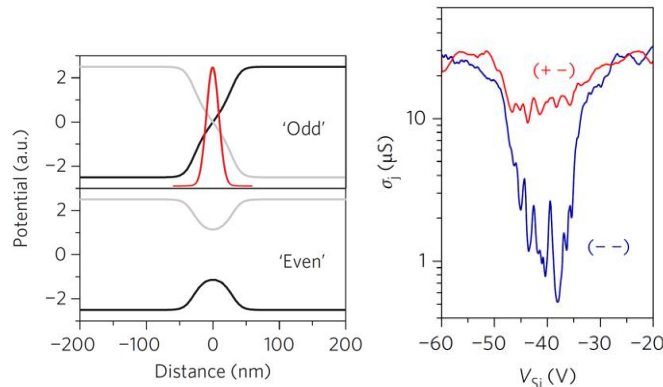
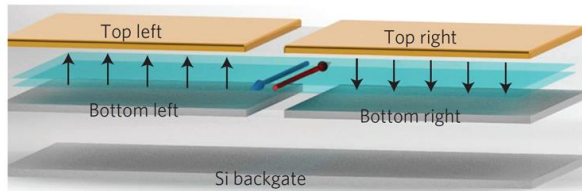
Creation of different shapes

- Initial site
- Non-equilibrium site
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Jiang *et al.*, *Nat. Nano. Letters* (2018)



Double gating



Design of the double gate device and measurements

- lithography limitations,
- MFP up to 200 nm,
- resistance close to $\frac{h}{4e^2}$, larger,
- valley valve and beam splitter, 4 gate structure.

Li *et al.*, *Nat. Nano.* **11**, 1060–1065 (2016)

Jing *et al.*, arXiv (2018)

Conclusion

I Possibility to define ballistic transport channels could lead to **low power dissipation devices**.

II Prospective applications in fields of **valleytronics** and very recently suggested **layertronics**.

III Approach is **applicable to different materials** and structures.

Is there a **possibility to control spin** in similar manner in TMDC-s, with strong spin-orbit coupling?

Electronic transport in 2D Materials



GRAPHENE FLAGSHIP

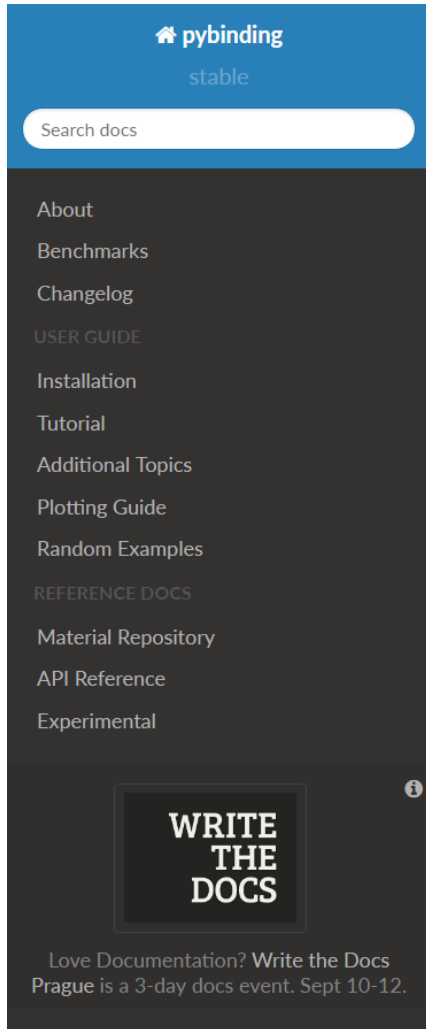
CMT

Condensed Matter Theory

cmt.uantwerpen.be

Bonus

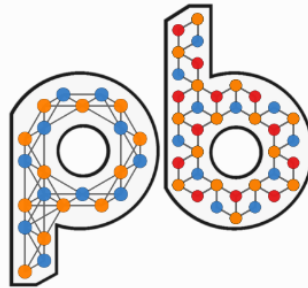
docs.pybinding.site



The screenshot shows the navigation menu of the pybinding website. At the top, there is a blue header with the pybinding logo and the word "stable". Below this is a search bar labeled "Search docs". The main menu is dark grey and contains several categories: "About", "Benchmarks", "Changelog", "USER GUIDE", "Installation", "Tutorial", "Additional Topics", "Plotting Guide", "Random Examples", "REFERENCE DOCS", "Material Repository", "API Reference", and "Experimental". At the bottom of the menu, there is a "WRITE THE DOCS" button and a promotional message: "Love Documentation? Write the Docs Prague is a 3-day docs event. Sept 10-12."

Docs » Tight-binding package for Python

[Edit on GitHub](#)



Pybinding is a scientific Python package for numerical tight-binding calculations in solid state physics. If you're just browsing, the [Tutorial](#) section is a good place to start. It gives a good overview of the most important features with lots of code examples.

As a very quick example, the following code creates a triangular quantum dot of bilayer graphene and then applies a custom asymmetric strain function:

```
import pybinding as pb
from pybinding.repository import graphene

def asymmetric_strain(c):
    @pb.site_position_modifier
    def displacement(x, y, z):
        ux = -c/2 * x**2 + c/3 * x + 0.1
        uy = -c*2 * x**2 + c/4 * x
        return x + ux, y + uy, z
    return displacement

model = pb.Model(
    graphene.bilayer(),
    pb.regular_polygon(num_sides=3, radius=1.1),
    asymmetric_strain(c=0.42)
)
model.plot()
```

