Hofstadter's Fractal Energy Spectrum in Twisted Bilayer Graphene

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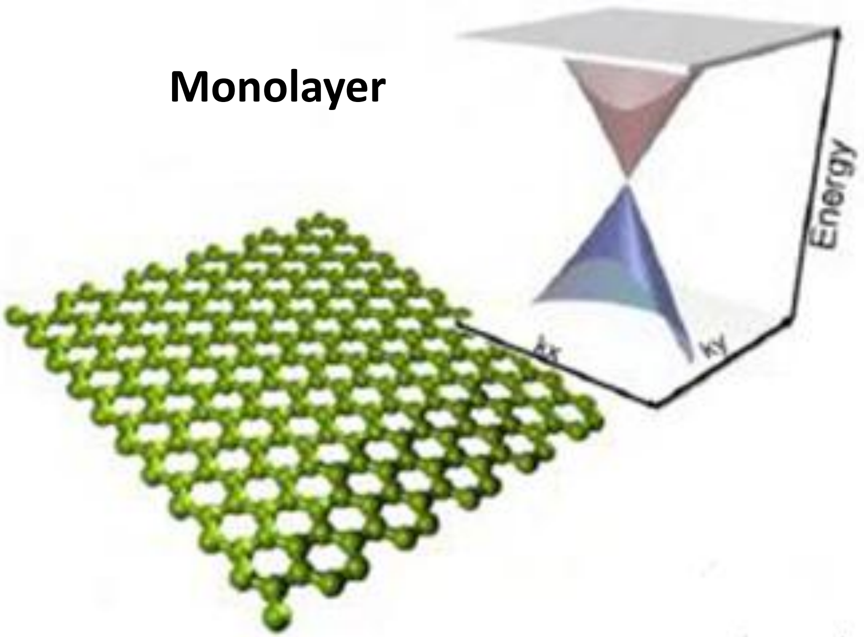
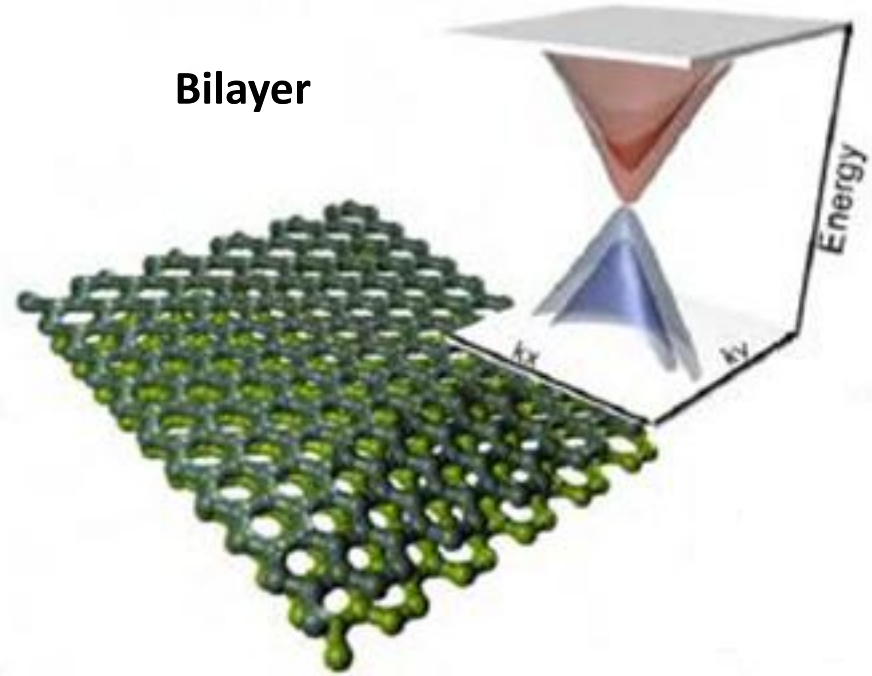
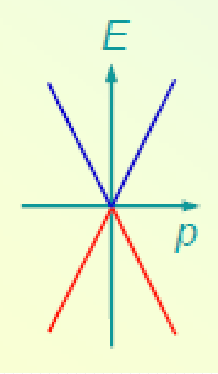
Band Structure of Monolayer and Bilayer Graphene

Monolayer

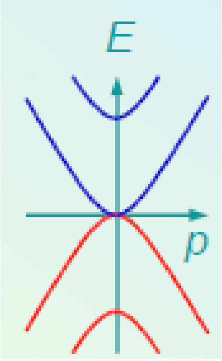


Bilayer



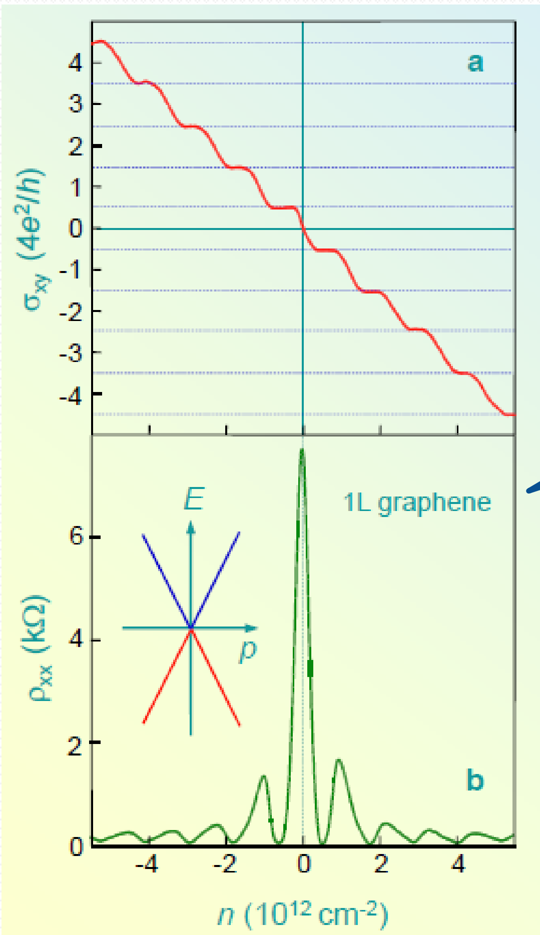


$$E = \pm \hbar v_f k$$



$$E = \pm \frac{\gamma_1}{2} \pm \sqrt{(\hbar v_f k)^2 + (\frac{\gamma_1}{2})^2}$$

Landau Levels of Monolayer and Bilayer Graphene



$$\varepsilon_N = \pm v_F \sqrt{2e\hbar BN}$$

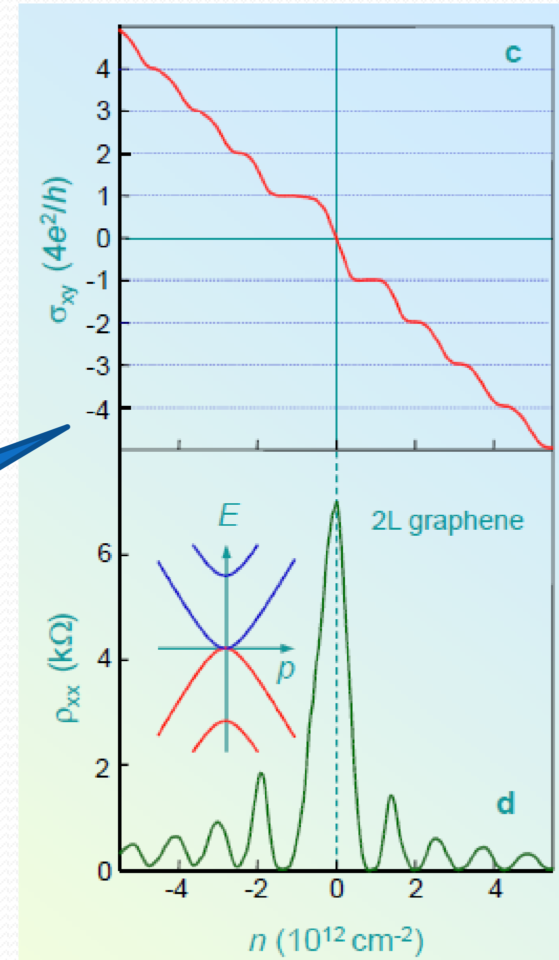
$$v_F = (\sqrt{3}/2)\gamma_0 a/\hbar$$

$$\sigma_{xy} = \pm 4\left(N + \frac{1}{2}\right)\frac{e^2}{h}$$

$$\varepsilon_N = \pm \hbar\omega_c \sqrt{N(N-1)}$$

$$\omega_c = eB/m$$

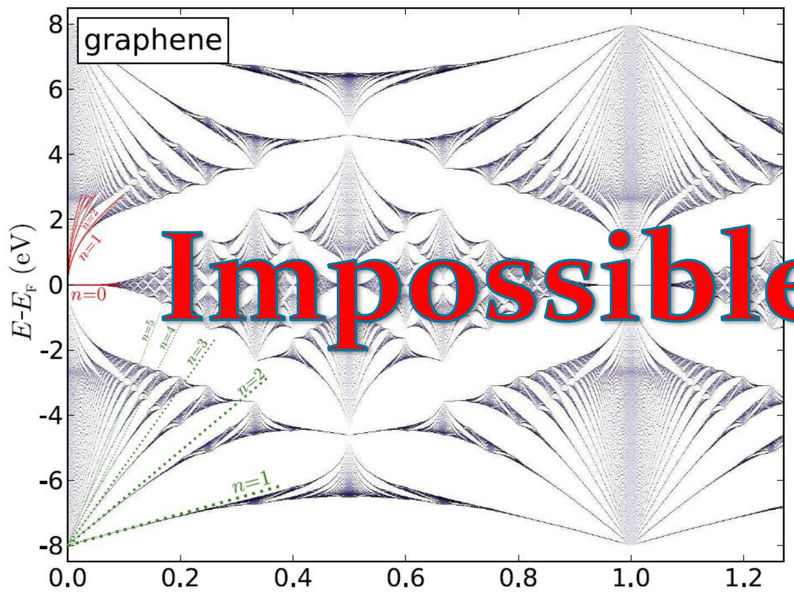
$$\sigma_{xy} = \pm 4N\frac{e^2}{h}$$



K. S. Novoselov, Nature Phys. 2, 177 (2006)

Hofstadter Butterflies of of Monolayer and Bilayer Graphene

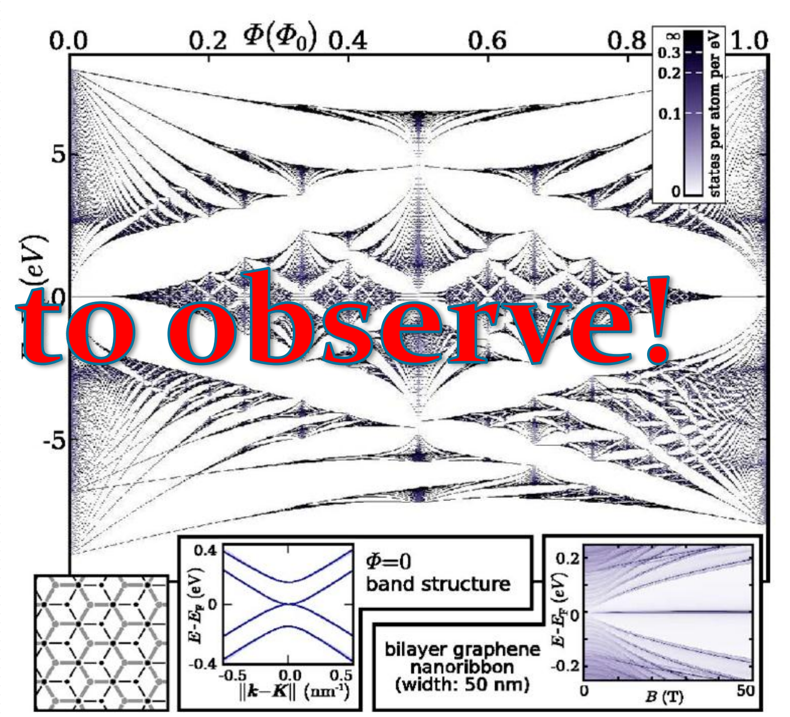
monolayer



ϕ/ϕ_o

N. Nemec *et al*.
Phys. Rev. B 74, 165411 (2006)

bilayer



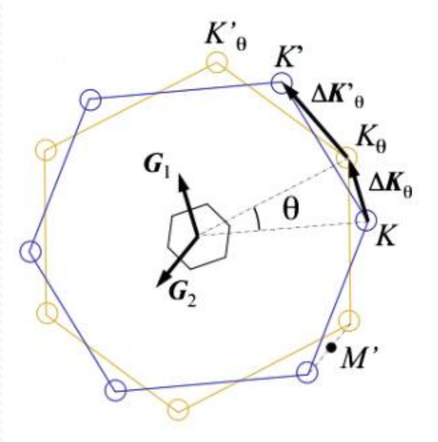
N. Nemec *et al*.
Phys. Rev. B 75, 201404 (R) (2007)

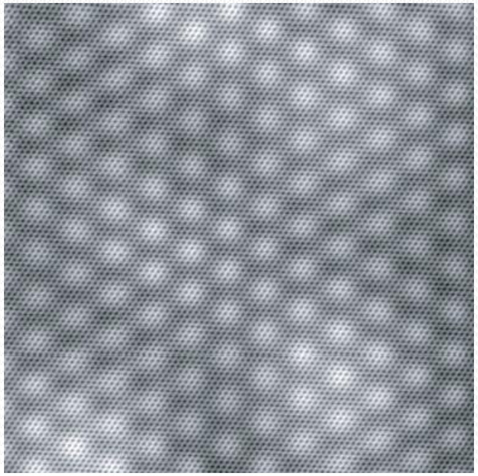
Impossible to observe!

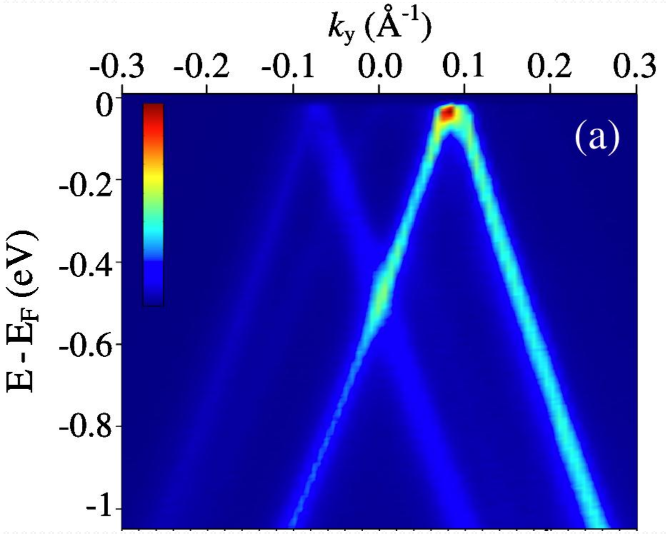
$$S = \frac{3\sqrt{3}}{2} a^2$$

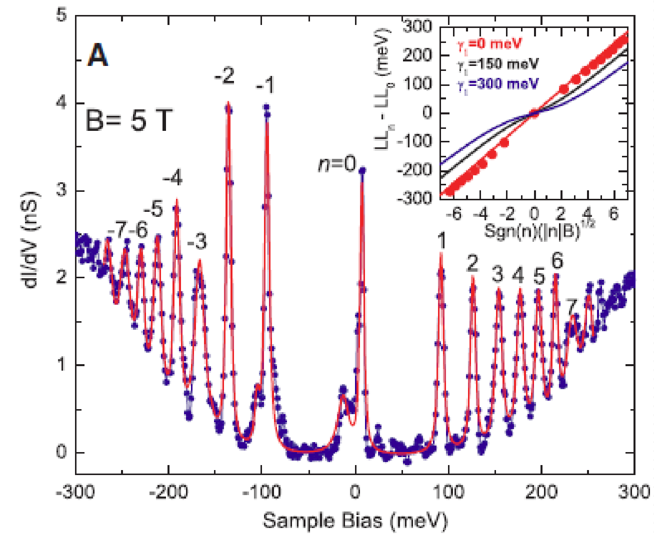
$\phi/\phi_0 = 1$, B=79098 T

Decoupling Behavior of Multilayer Epitaxial Graphene





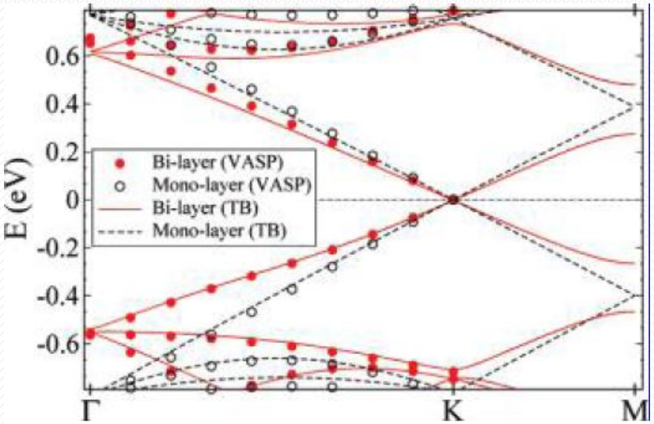


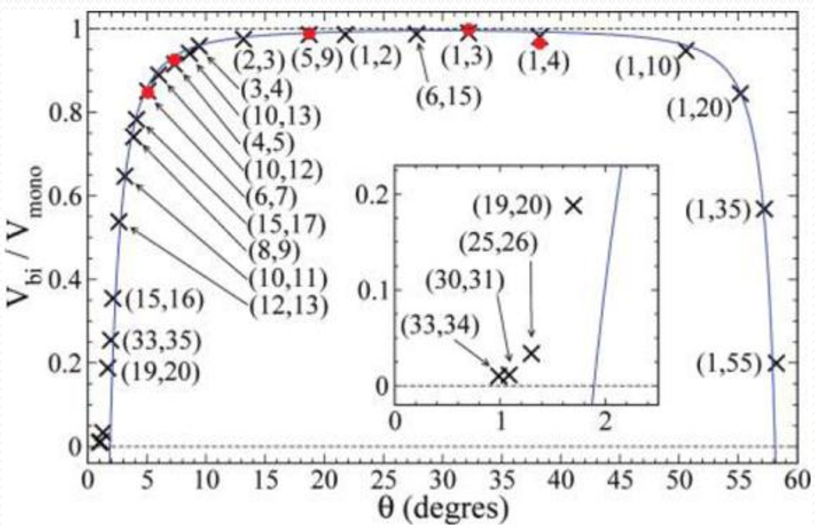


M. Sprinkle *et al.*
Phys. Rev. Lett. 103, 226803 (2009)

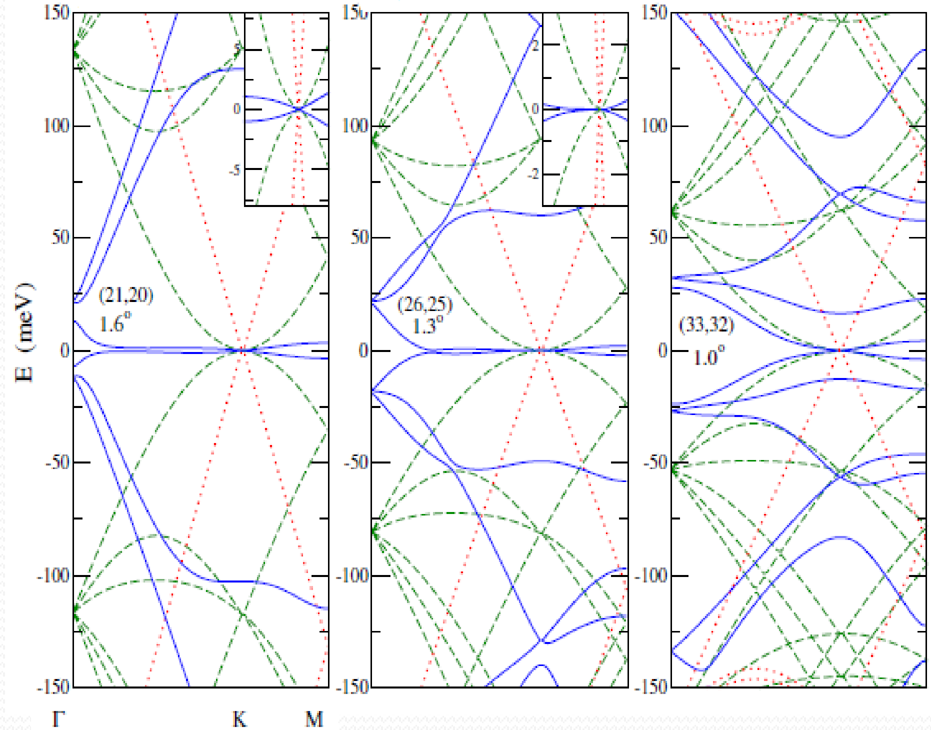
D. L. Miller *et al.*
Science 324, 924 (2009)

Band Structure of Twisted Bilayer Graphene





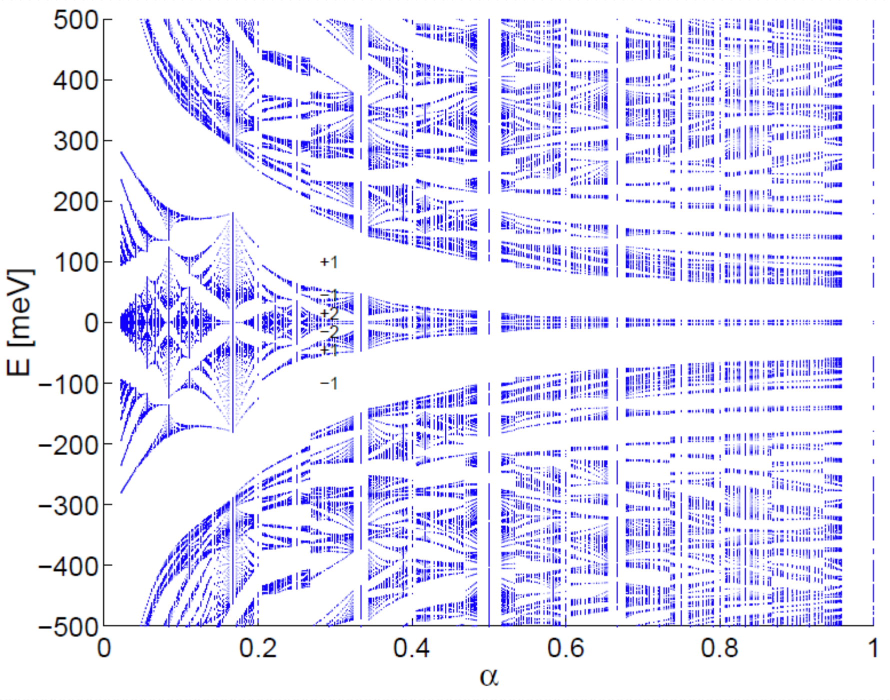
G. T. de Laissardiere *et al.*
Nano Lett. 10, 804 (2010)



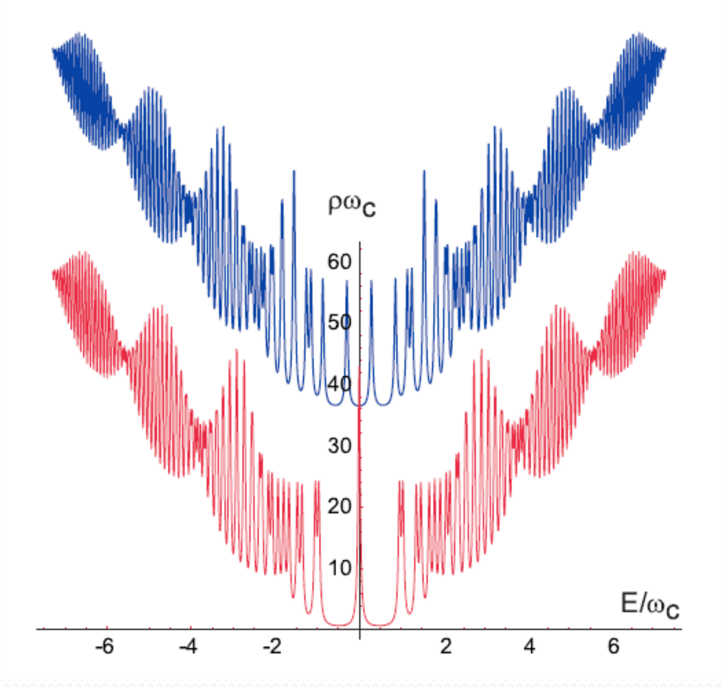
E. Suárez Morell *et al.*
Phys. Rev. B 82, 121407(R) (2010)

Recent Results of Twisted Bilayer Graphene in "Low" Magnetic Field

Morie Butterfly



Dirac Comb



R. Bistritzer and A.H. MacDonald
arXiv:1101.2606v1

M. Kindermann and E.J. Mele
arXiv:1106.0204v1

Motivation

- How do the electronic properties of twisted bilayer graphene change with the twist angle?
- How do the LLs evolve as the twist angle changes?
- Will there be a difference between twisted bilayer graphene with commensurate and incommensurate angles?

Lanczos Recursive Method

Real space Hamiltonian (Hermitian matrix)

$$H = \sum_{i,j} t_{ij} \exp\left(\frac{ie}{\hbar}\int_i^j \vec{A}\cdot d\vec{l}\right) a_i^+ a_j \qquad \vec{A} = (0, Bx)$$

Construct a new orthogonal basis

$$\{|\Phi_0\rangle, |\Phi_1\rangle, |\Phi_2\rangle \cdots |\Phi_N\rangle\}$$

$|\Phi_0\rangle$ is the initial state localized at one atom site

N is the total number of atoms

$$|\Phi_0\rangle$$

$$a_0 = \langle\Phi_0|H|\Phi_0\rangle$$

$$|\tilde{\Phi}_1\rangle = b_1|\Phi_1\rangle = H|\Phi_0\rangle - a_0|\Phi_0\rangle$$

$$a_1 = \langle\Phi_1|H|\Phi_1\rangle \qquad b_1 = \sqrt{\langle\tilde{\Phi}_1|\tilde{\Phi}_1\rangle}$$

$$|\tilde{\Phi}_2\rangle = b_2|\Phi_2\rangle = H|\Phi_1\rangle - a_1|\Phi_1\rangle - b_1|\Phi_0\rangle$$

$$a_1 = \langle\Phi_2|H|\Phi_2\rangle \qquad b_2 = \sqrt{\langle\tilde{\Phi}_1|\tilde{\Phi}_2\rangle}$$

…………

Recursive relation

$$|\tilde{\Phi}_{N+1}\rangle = b_{N+1}|\Phi_{N+1}\rangle = H|\Phi_N\rangle - a_N|\Phi_N\rangle - b_N|\Phi_{N-1}\rangle$$

$$a_N = \langle\Phi_N|H|\Phi_N\rangle \qquad b_N = \sqrt{\langle\tilde{\Phi}_N|\tilde{\Phi}_N\rangle}$$

Hamiltonian in the new basis

$$H_{ij} = \langle \Phi_i | H | \Phi_j \rangle \qquad H = \begin{pmatrix} a_0 & b_1 & 0 & \cdots \\ b_1 & a_1 & b_2 & \cdots \\ 0 & b_2 & a_2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Real space Green's function at the initial state (continued fraction expansion)

$$\langle \Phi_0 | G^r(E+i\eta) | \Phi_0 \rangle = \cfrac{1}{E+i\eta-a_0-\cfrac{b_1^2}{E+i\eta-a_1-\cfrac{b_2^2}{E+i\eta-a_2-\cdots}}}$$

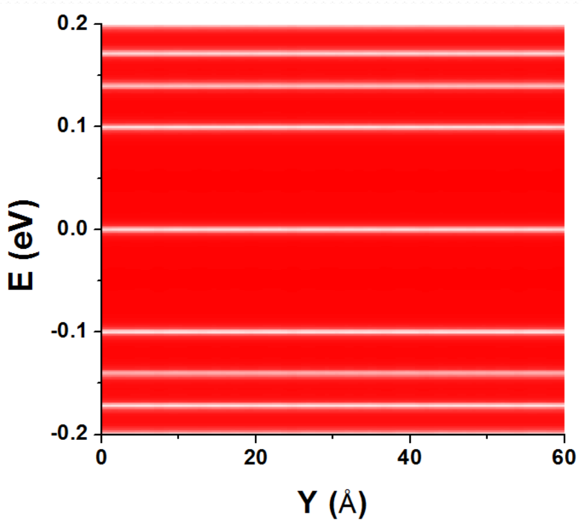
$$\cdots$$

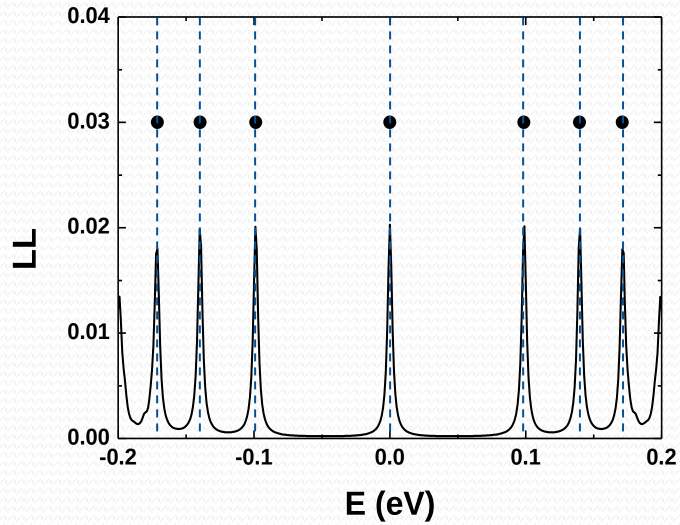
$$LDOS = -\frac{1}{\pi}\,\mathrm{Im}\,G^r(E+i\eta)$$

140nm×140nm, over 1.5million atoms!

Landau Levels of Monolayer and Bilayer Graphene

Monolayer graphene

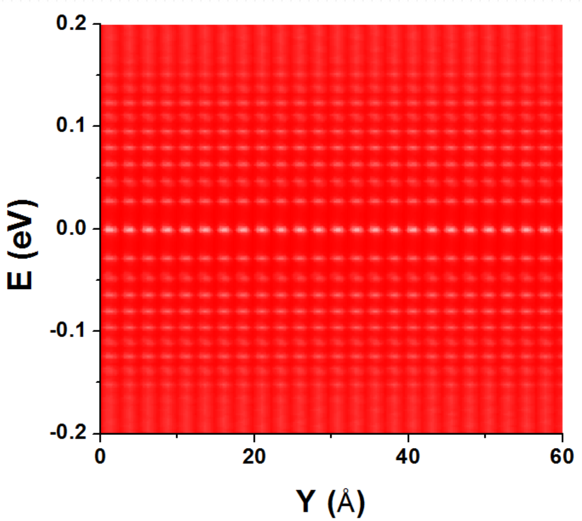


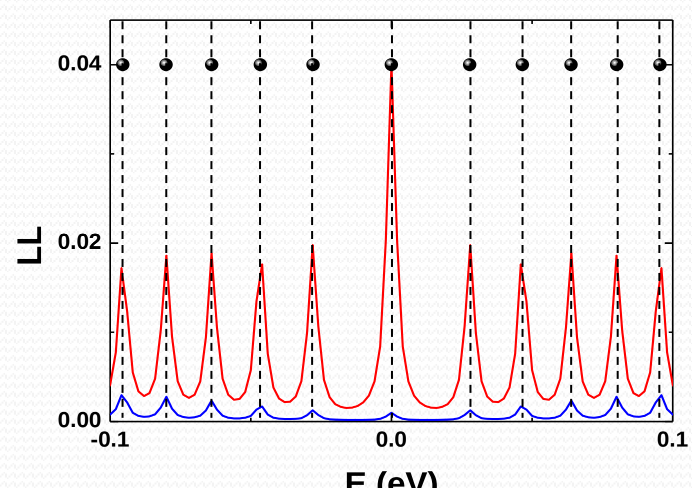


$$E_n = \mathrm{sgn}(n)\Delta\sqrt{|n|}$$

$$\Delta = \sqrt{2eBv_F^2\hbar}$$

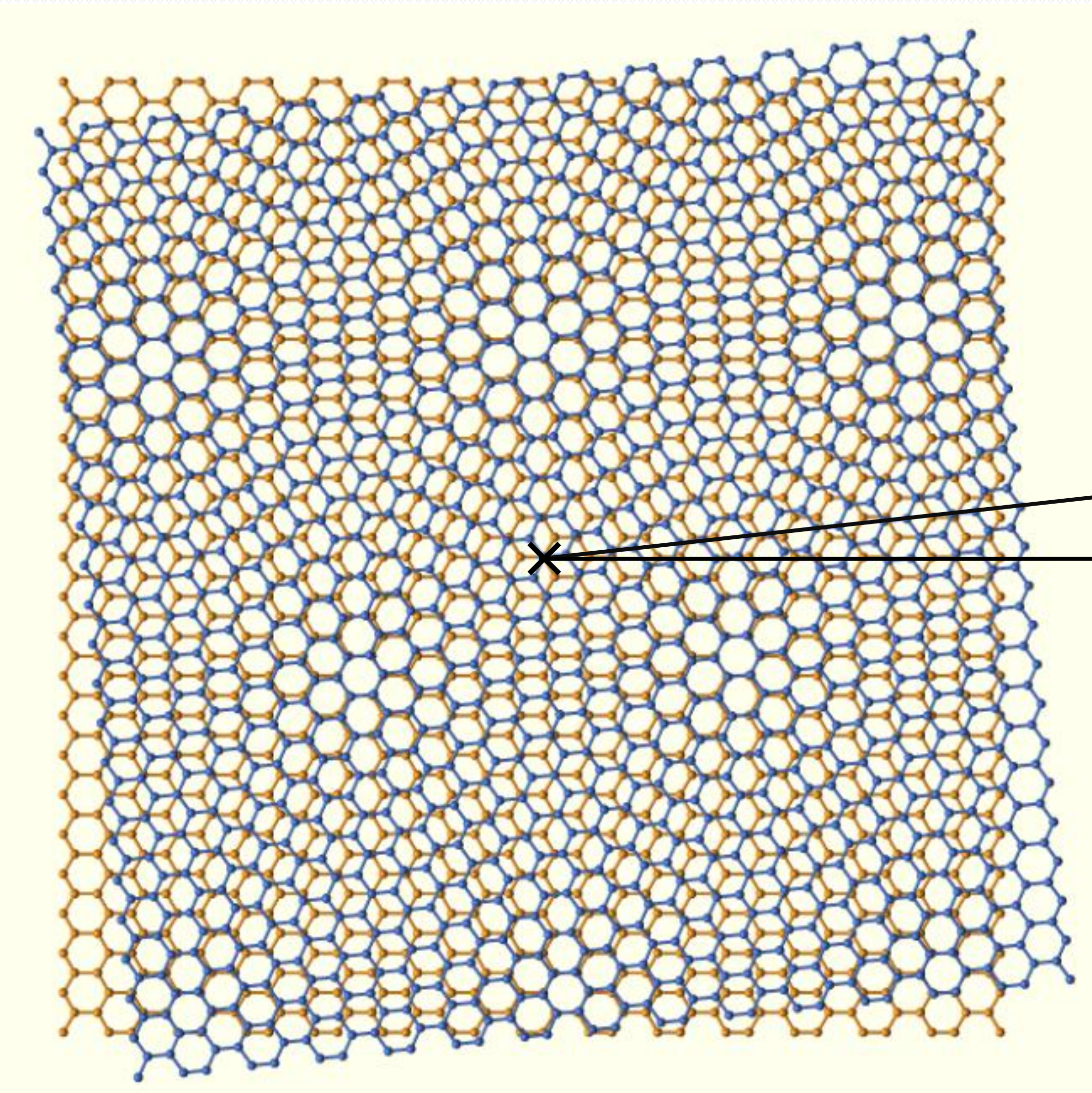
AB bilayer graphene





$$E_n = \frac{\mathrm{sgn}(n)}{\sqrt{2}}\Big[(2|n|+1)\Delta^2 + \gamma_1^2 - \sqrt{\gamma_1^4 + 2(2|n|+1)\Delta^2\gamma_1^2 + \Delta^4}\Big]^{1/2}$$

Twisted Bilayer Graphene



Starting from AB stacking bilayer graphene, bottom layer is fixed and top layer is twisted.

Twist center is at A atom in the top layer with a neighboring B atom in the bottom layer.

θ

Commensurate angle

$$\theta = \cos^{-1}\left(\frac{3q^2 - p^2}{3q^2 + p^2}\right)$$

S. Shallcross *et al.*
Phys. Rev. B 81, 1 (2010)

Other θ's are incommensurate angles

Tight-binding Parameterization

$$H = \sum_{\mu,\nu=1,2} \sum_{l,j} t_{\mu l,\nu j} exp[\frac{ie}{\hbar}\int_{\vec{r}_{\mu l}}^{\vec{r}_{\nu j}} \vec{A}\cdot d\vec{l}]|\mu l\rangle\langle\nu j|$$

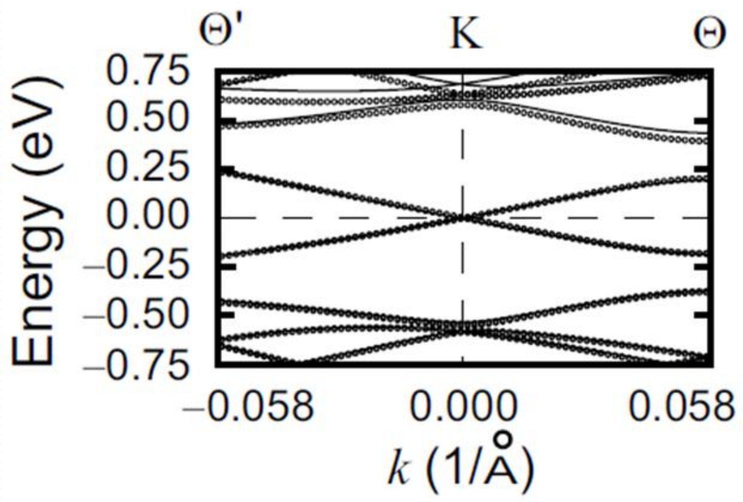
TB parameters are obtained by fitting the TB bands to reproduce first-principles band structures

$$t_{\mu l,\nu j} = \begin{cases} \gamma_1 exp[\lambda_1(1-|\vec{r}_{\mu l}-\vec{r}_{\nu j}|/a)] & (\mu=\nu) \\ \gamma_2 exp[\lambda_2(1-|\vec{r}_{\mu l}-\vec{r}_{\nu j}|/c)] & (\mu\neq\nu) \end{cases}$$

$a = 1.42\mathring{A}$ $\quad \gamma_1 = -2.7eV$ $\quad \lambda_1 = 3.15$

$c = 3.35\mathring{A}$ $\quad \gamma_2 = 0.48eV$ $\quad \lambda_2 = 7.42$

θ=3.89°



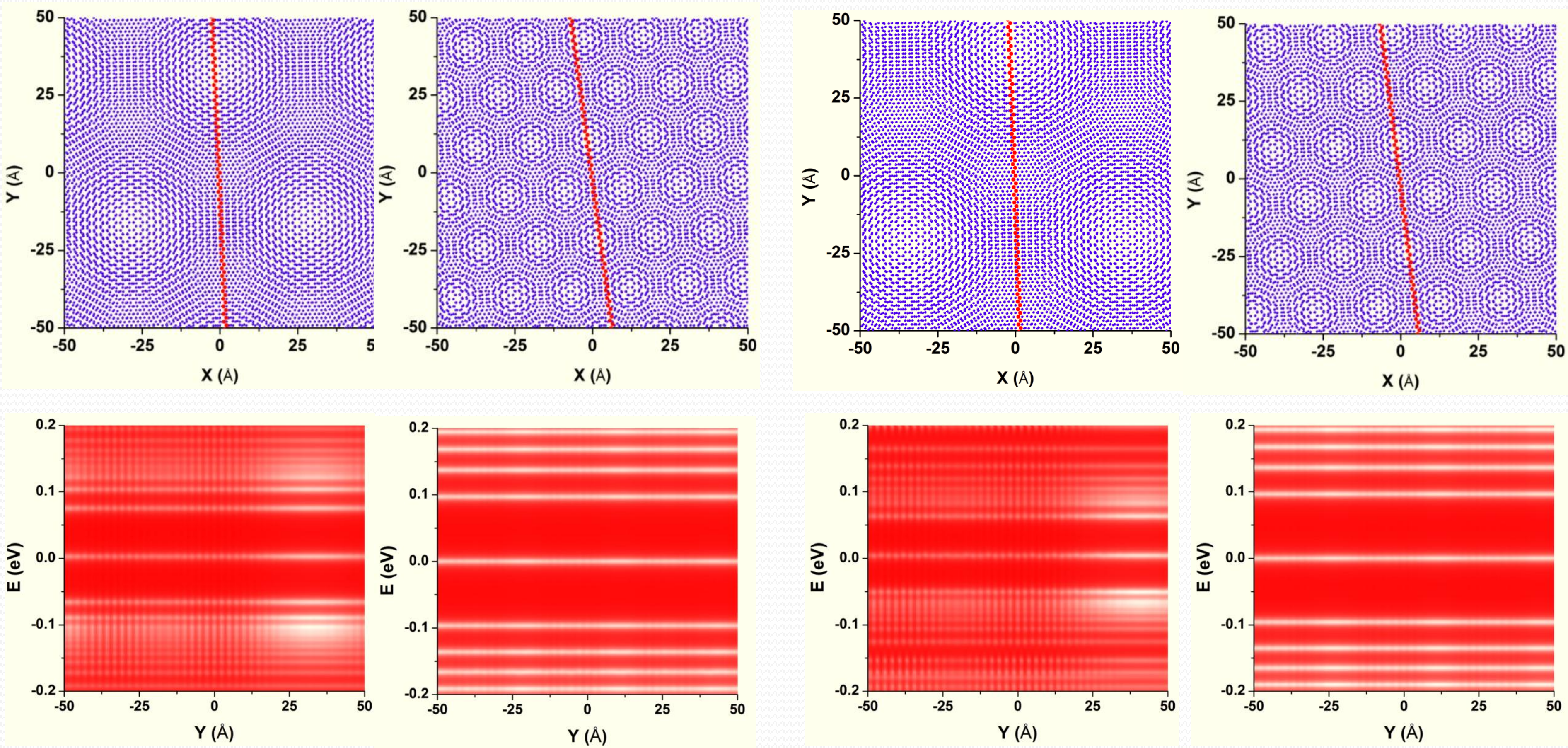
G. T. de Laissardiere *et al.*
Nano Lett. 10, 804 (2010)

Landau Levels as a Function of Position

Commensurate , B=10T

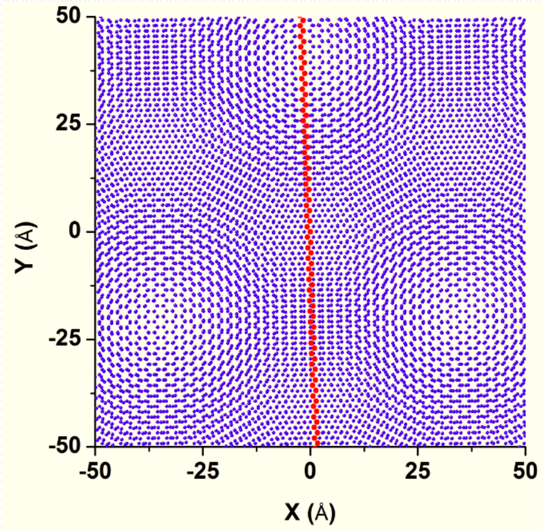
Incommensurate , B=10T

$\theta=2.4718^{o}$ **$\theta=7.56507^{o}$** **$\theta=2.0^{o}$** **$\theta=7.0^{o}$**

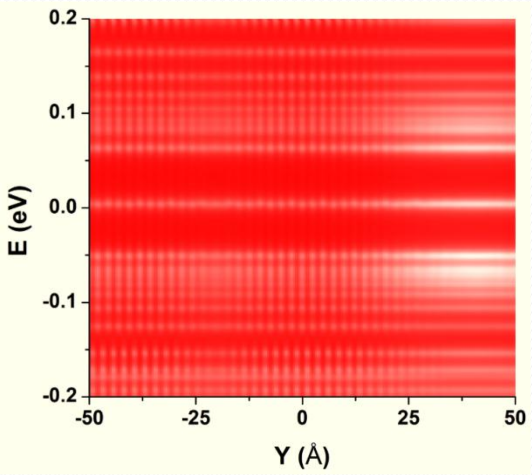


Landau Levels as a Function of Position

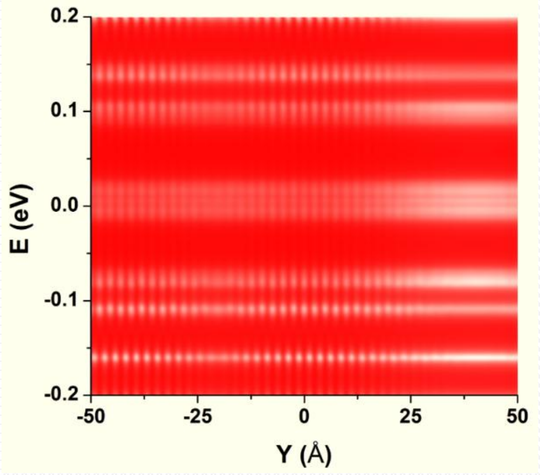
Incommensurate, θ=2.0°



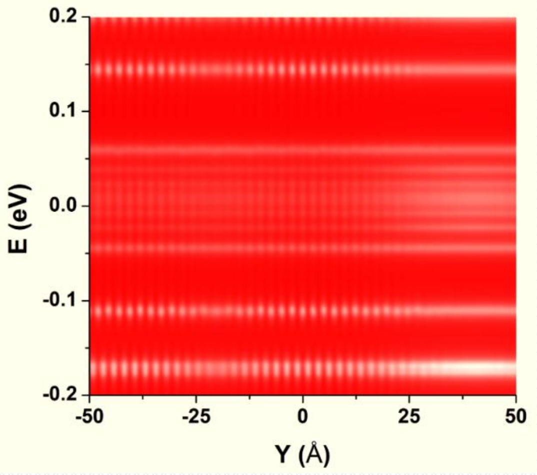
B=10T



B=30T

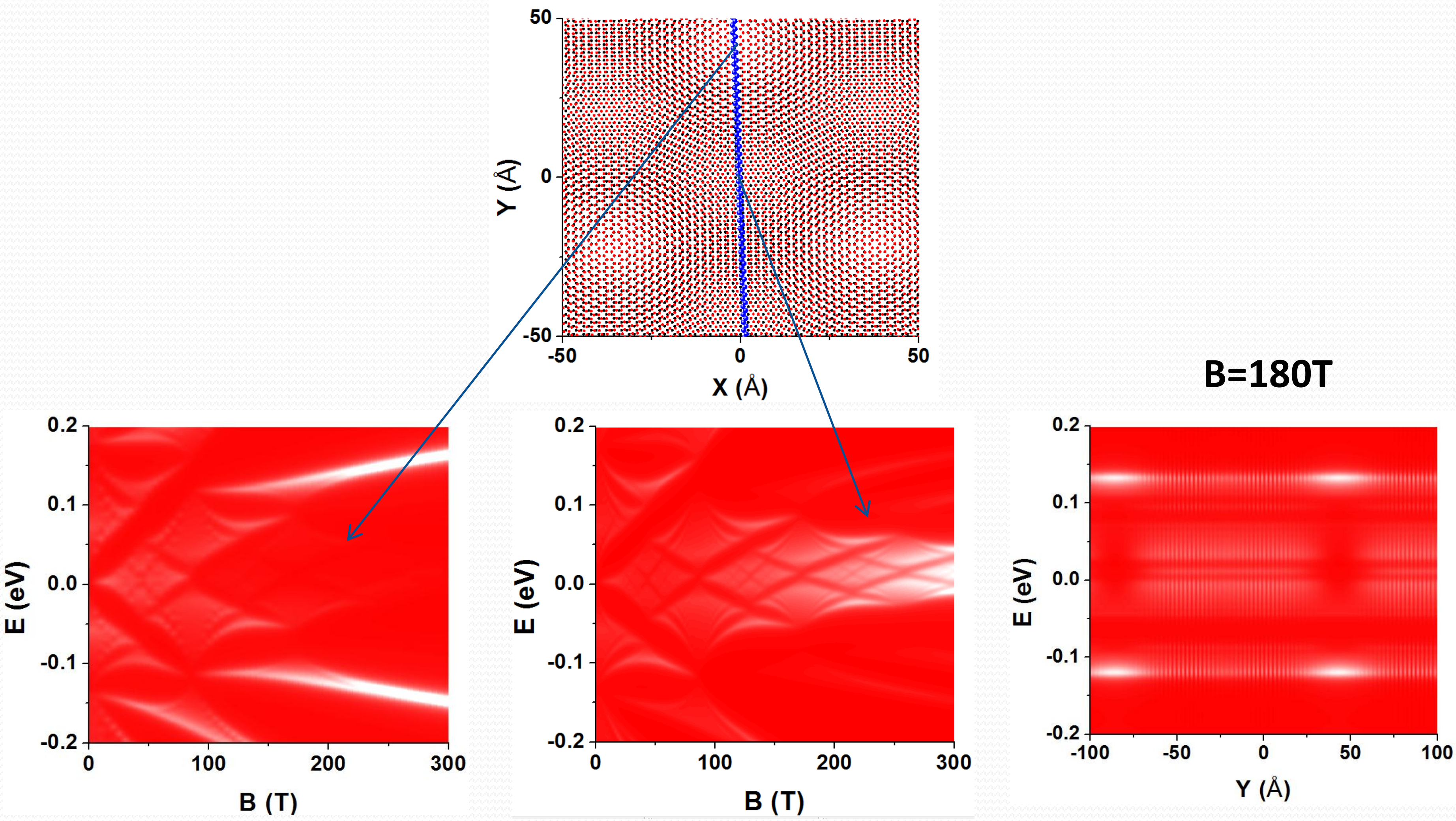


B=60T

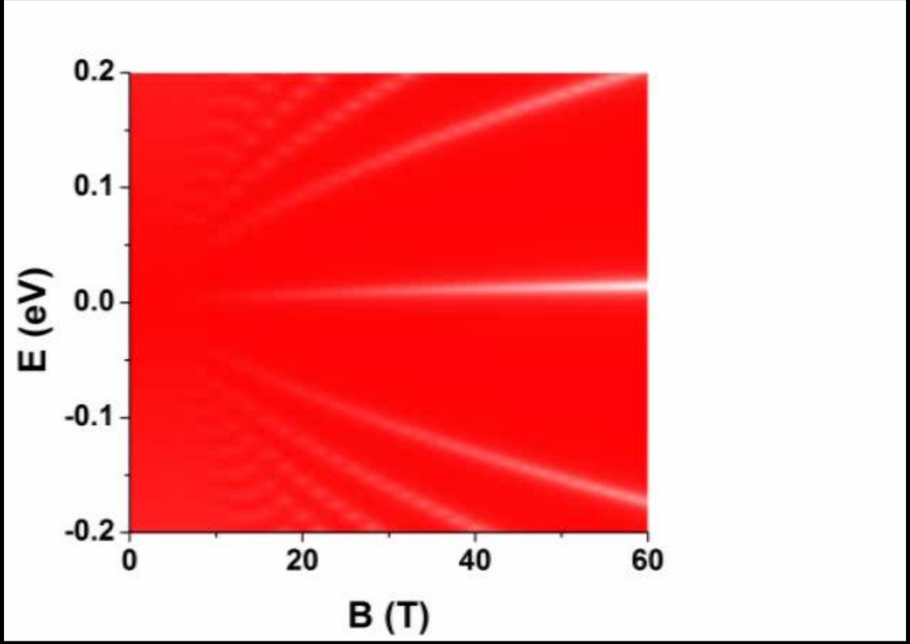


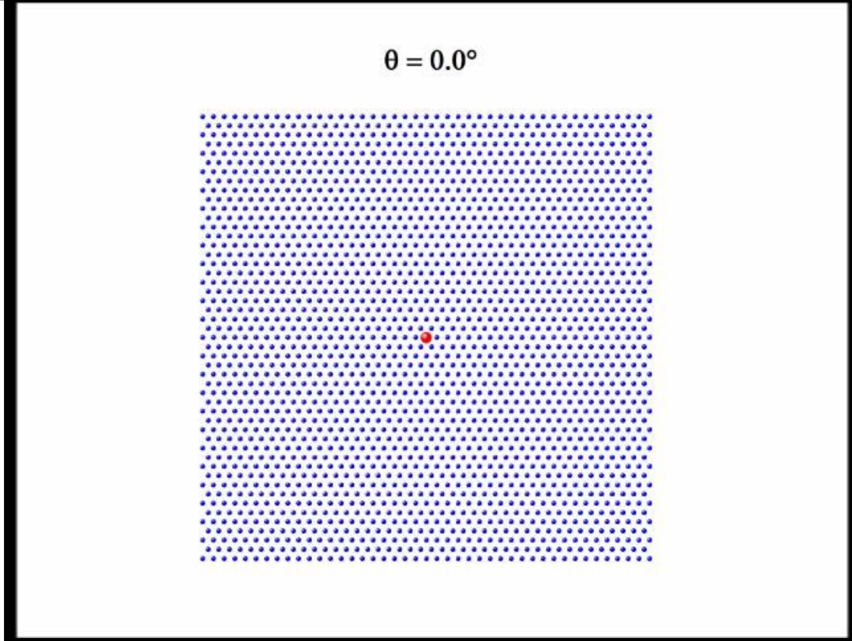
Landau Levels as a Function of Position

commensurate, θ=1.8901°

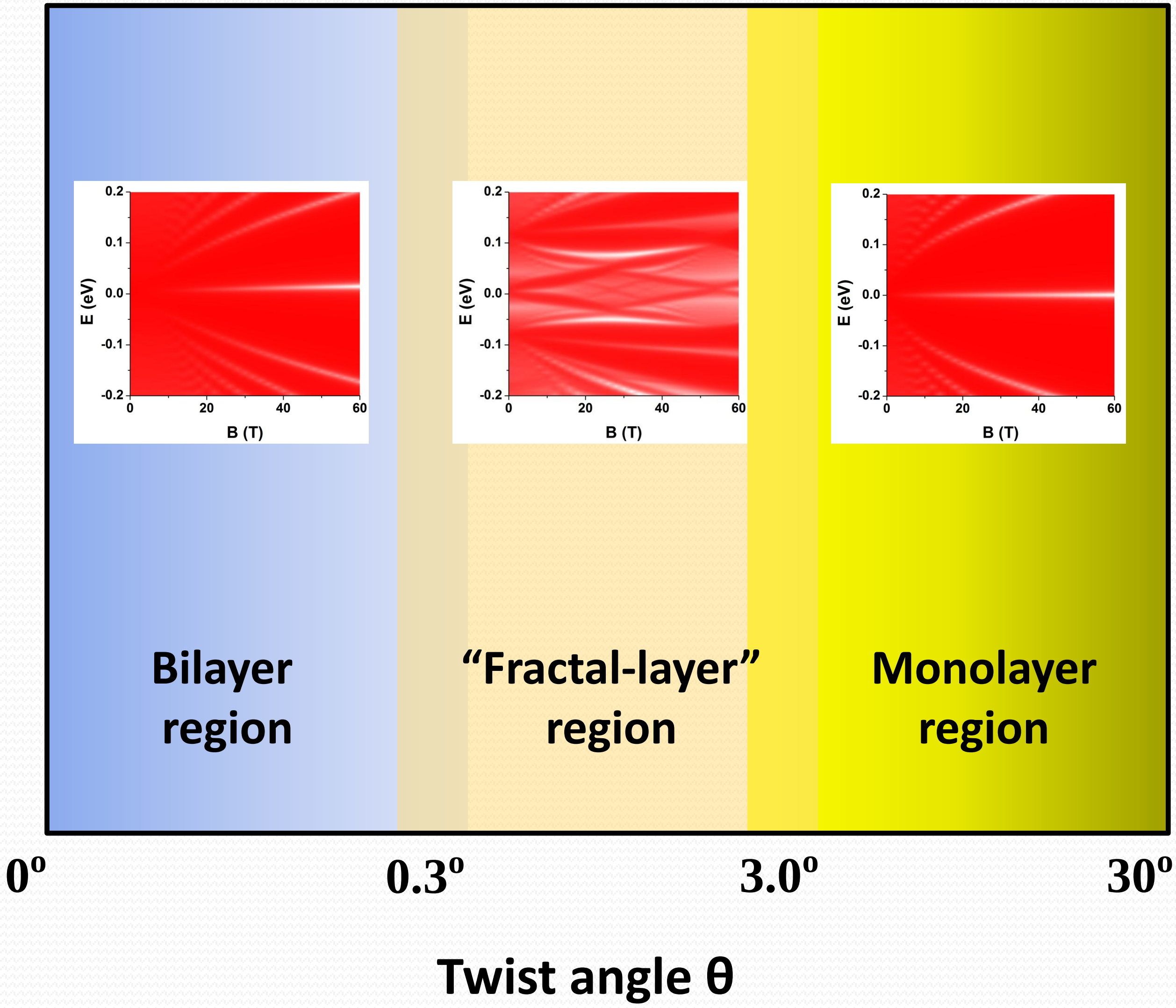


Landau Levels as a Function of Twist Angle



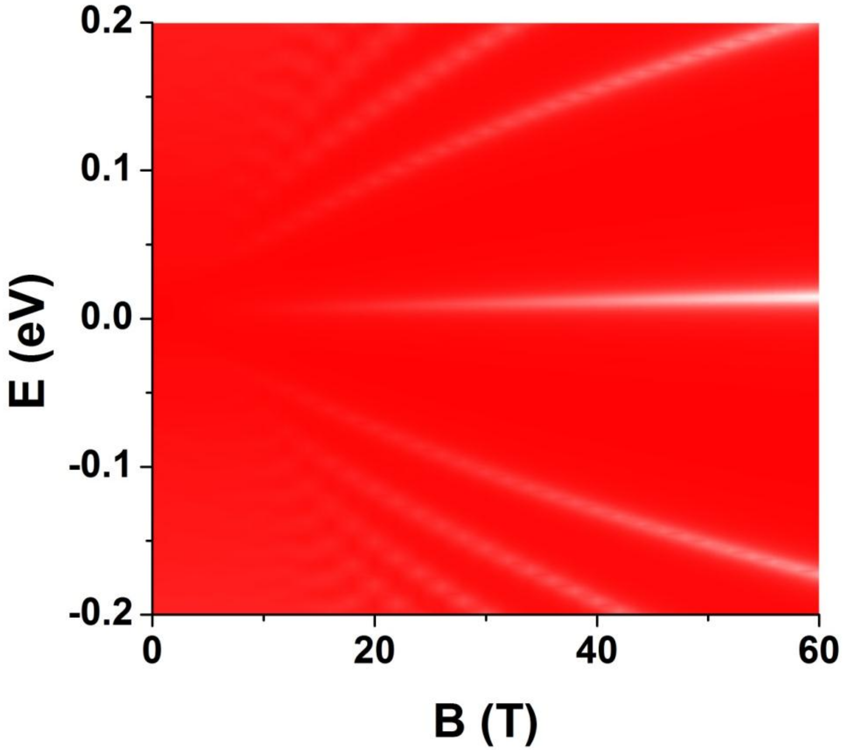


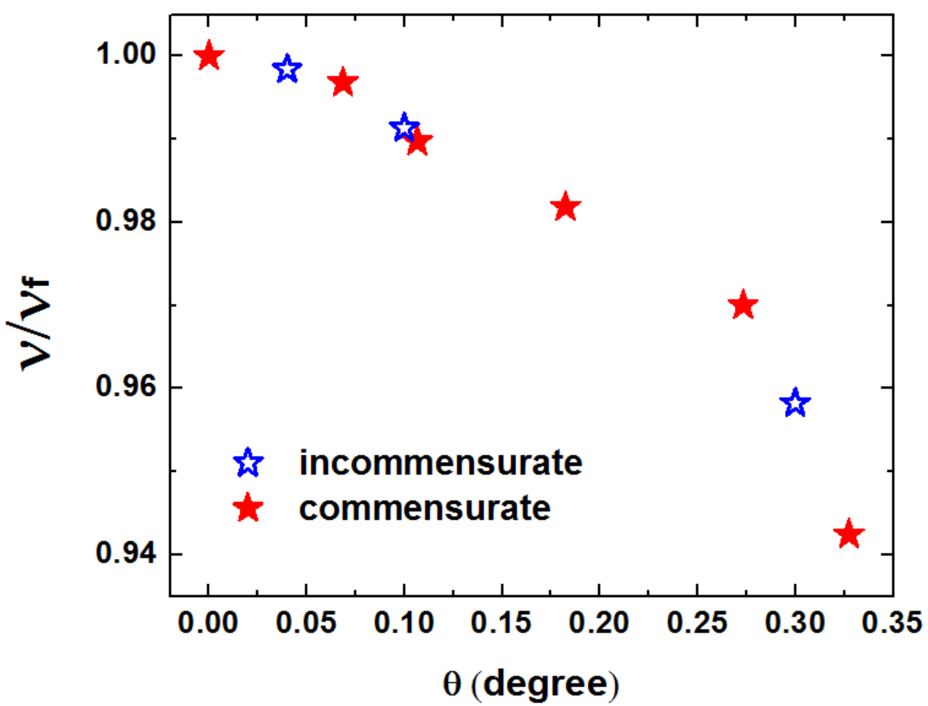
Laudau Levels of Twisted Bilayer Graphene



"Near-Zero" Twist Angles: Bilayer Graphene Region

Commensurate
θ=0.06853°



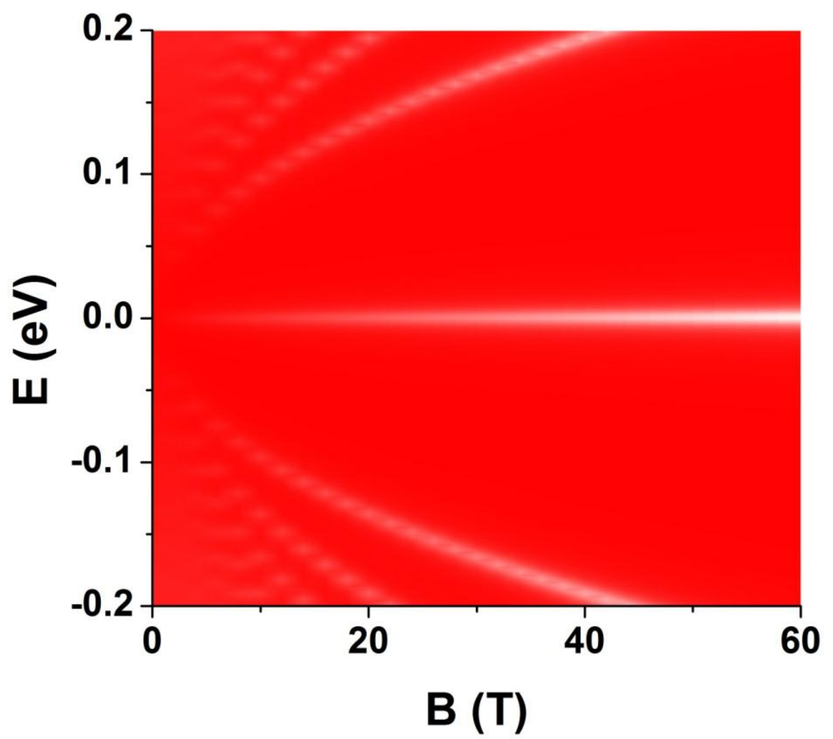


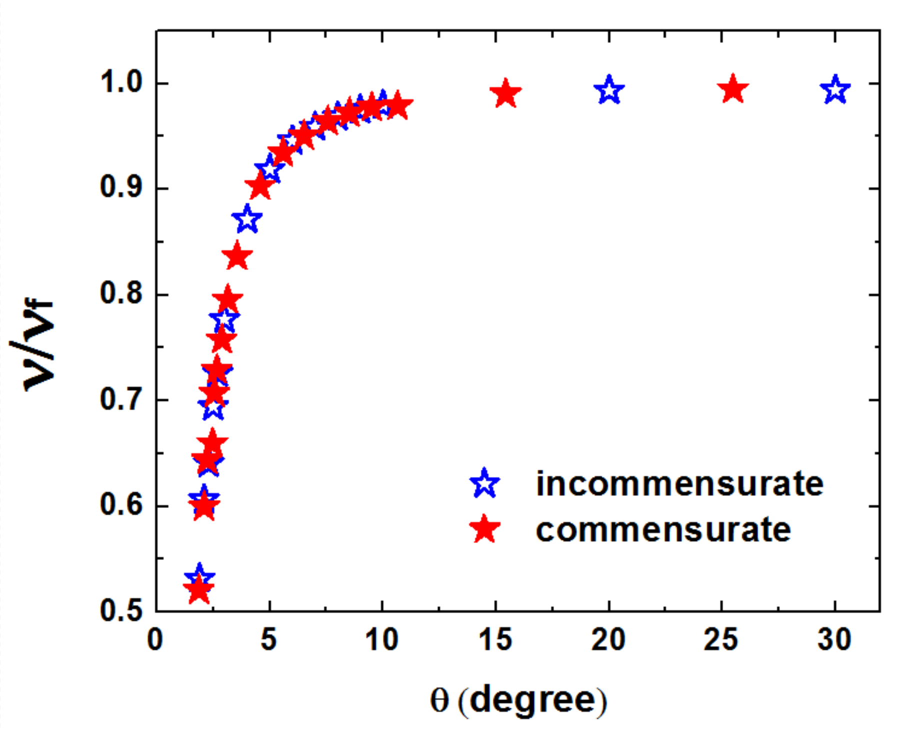
$$E_n = \frac{\mathrm{sgn}(n)}{\sqrt{2}}\left[(2|n|+1)\Delta^2 + \gamma_1^2 - \sqrt{\gamma_1^4 + 2(2|n|+1)\Delta^2\gamma_1^2 + \Delta^4}\right]^{1/2}$$

$$\Delta = \sqrt{2eBv_F^2\hbar}$$

Large Twist Angles: Monolayer Graphene Region

Commensurate
θ=7.56507°





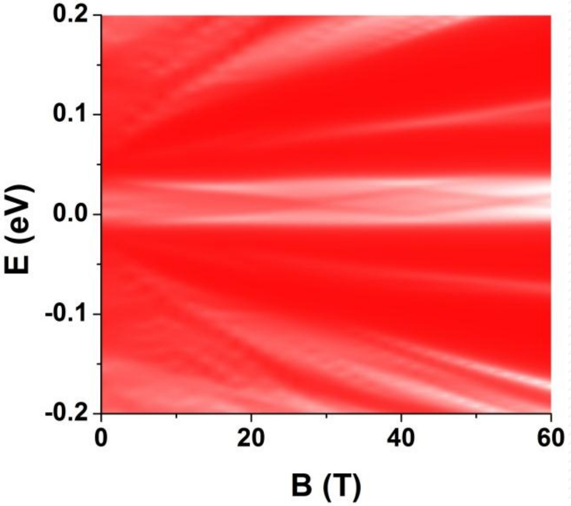
$$E_n = \mathrm{sgn}(n)\Delta\sqrt{|n|}$$

$$\Delta = \sqrt{2eBv_F^2\hbar}$$

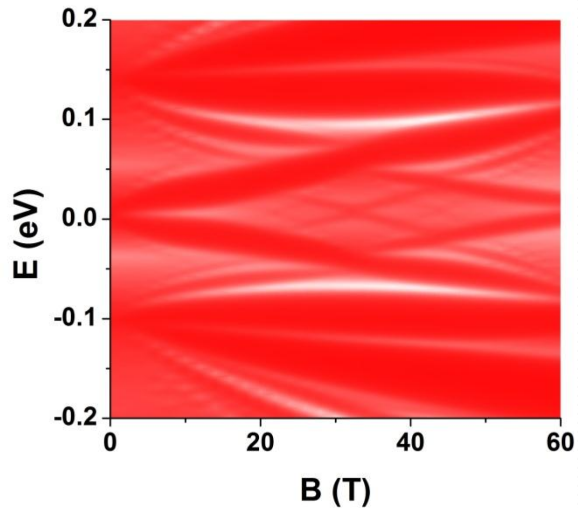
Small Twist Angles: “Fractional-layer” Region

Commensurate:

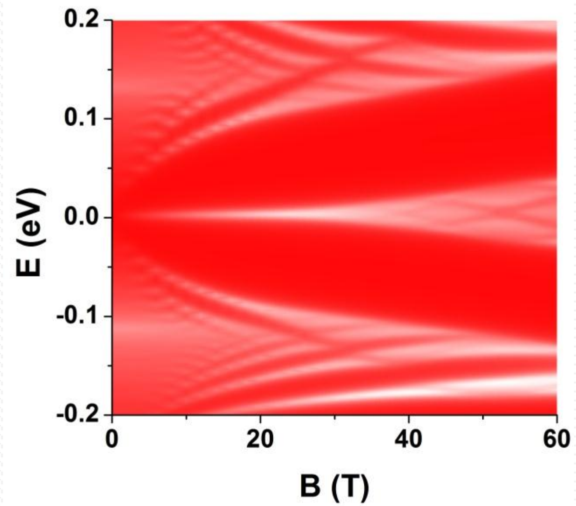
θ=1.06689°



θ=1.64996°

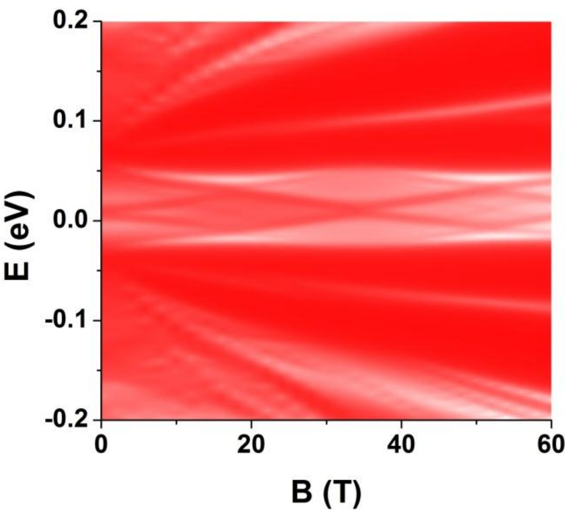


θ=2.56292°

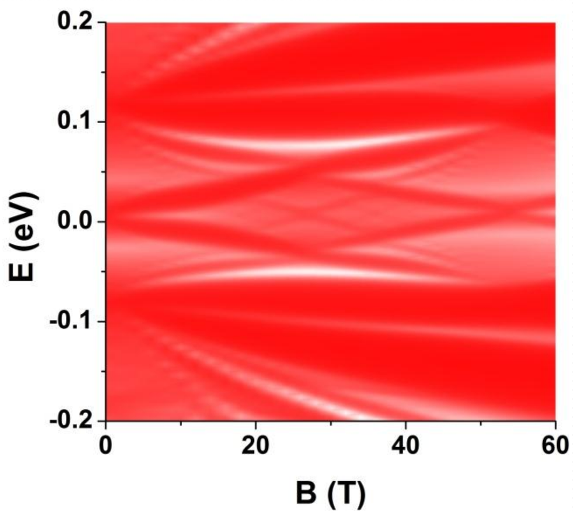


Incommensurate:

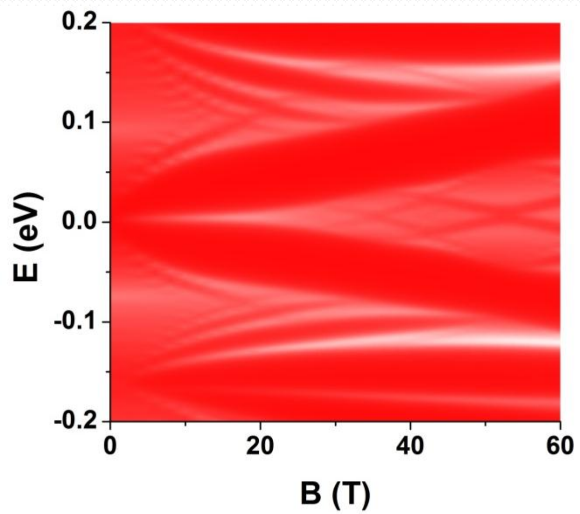
θ=1.2°



θ=1.5°

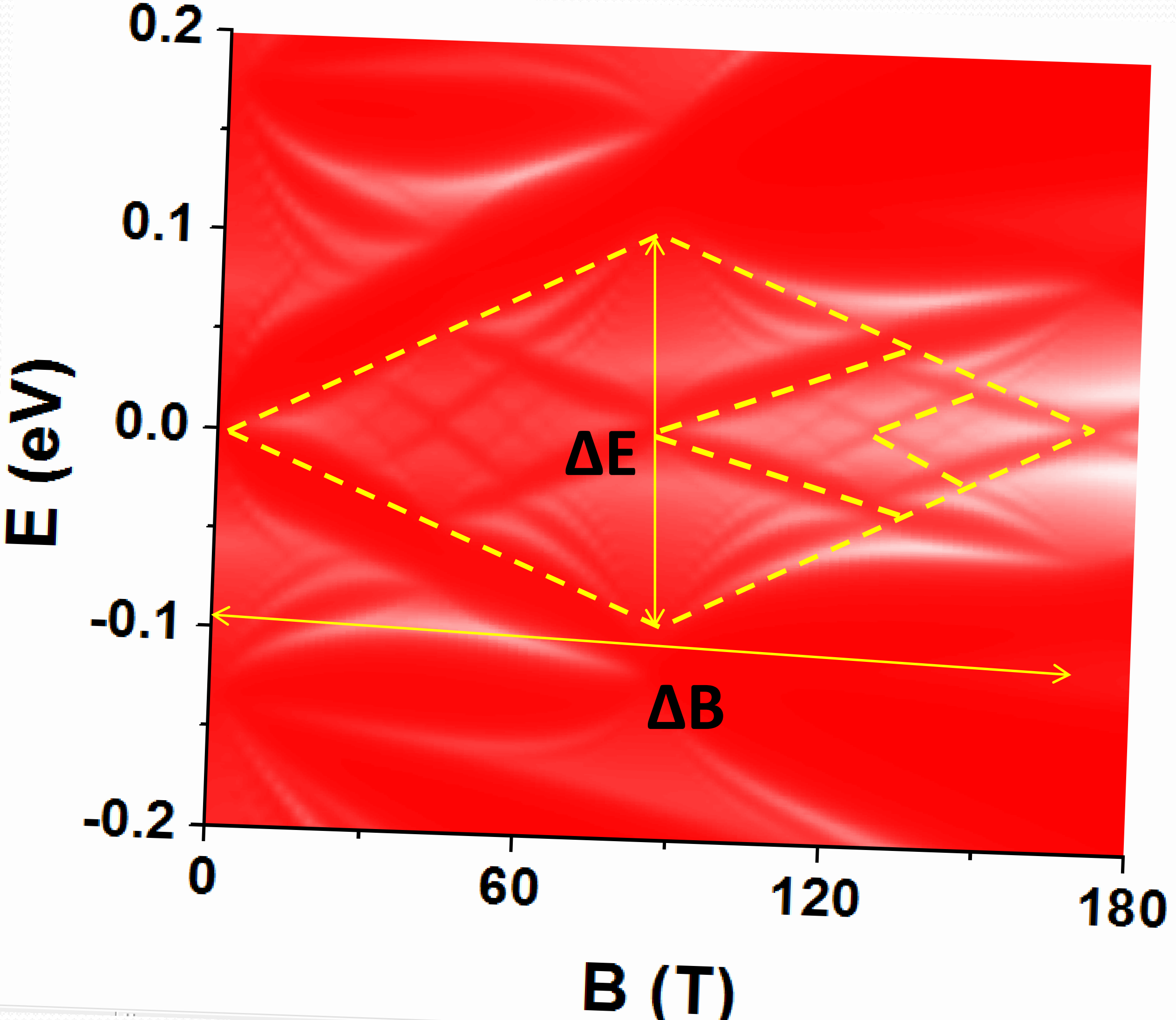


θ=2.1°



Fractal Spectra

Commensurate: θ=1.8901°



Conclusion

- Local LLs are independent of the lattice position for both commensurate and incommensurate twist angles in low magnetic field.

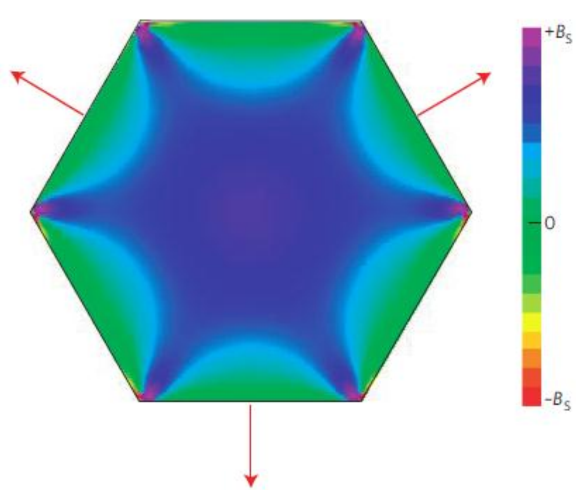
- The behavior of LLs can be classified into three regions depending on the twist angle.

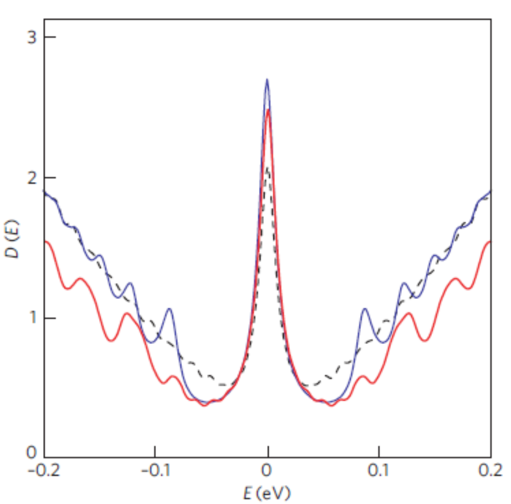
- LLs in the regions of near-zero and large twist angles are characterized by a renormalized Fermi velocity as bi- and mono-layer graphene, respectively.

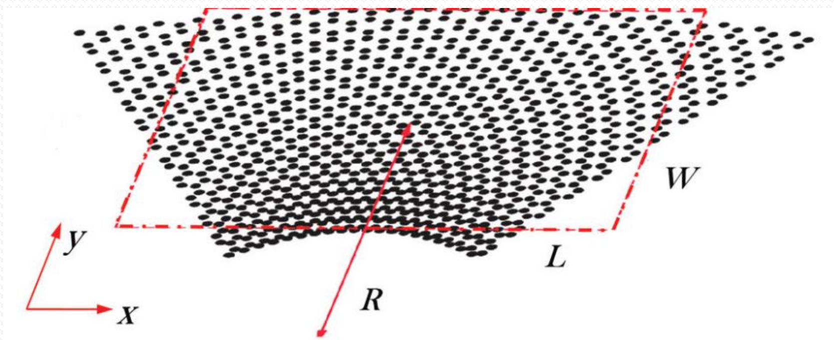
- In between, LLs show a complex fractional-layer behavior (Hofstadter butterfly) in a reasonably low magnetic field.

Pseudo Magnetic Field in Graphene Nanobubble

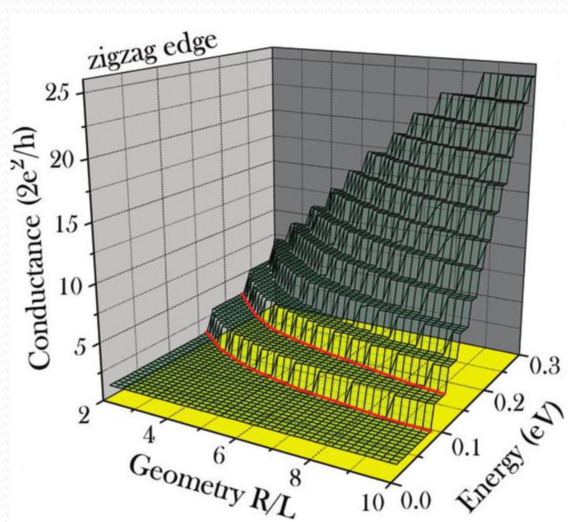
Strain-Induced Pseudo–Magnetic Fields







Strain field



$$\vec{A} = \frac{\beta}{a_0}\begin{pmatrix} u_{xx} - u_{yy} \\ -2u_{xy} \end{pmatrix}$$

$$\beta \approx \left.\frac{\partial \log(t)}{\partial \log(a)}\right|_{a=a_0}$$

$$\approx 2-3$$

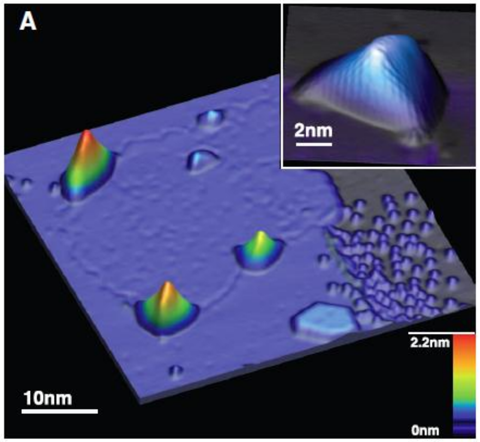
Filling factor

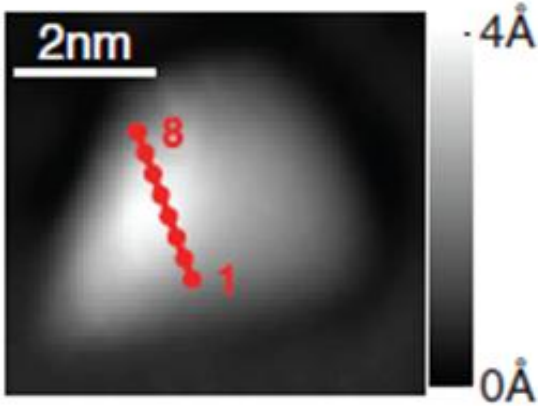
$$\nu = 2, 6, 10, \ldots = 4n + 2$$

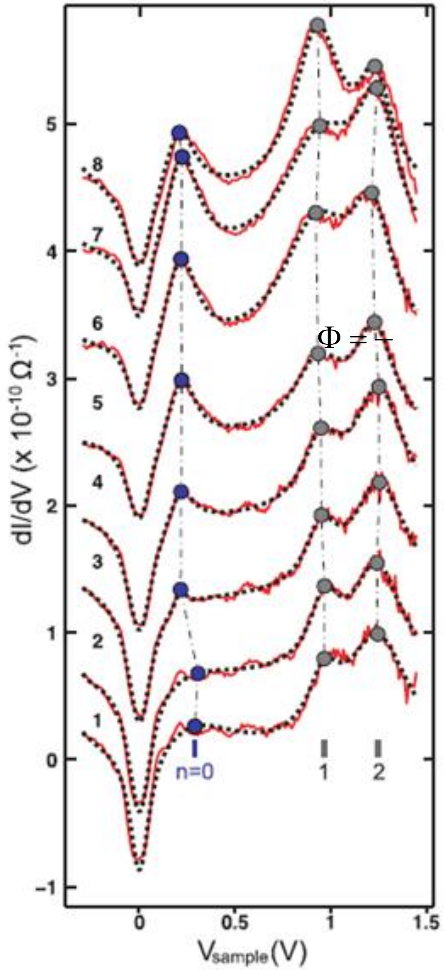
F. Guinea, *et al.*
Nature Phys. 6, 30 (2010)

Tony Low and F. Guinea
Nano Lett. 10, 3551 (2010)

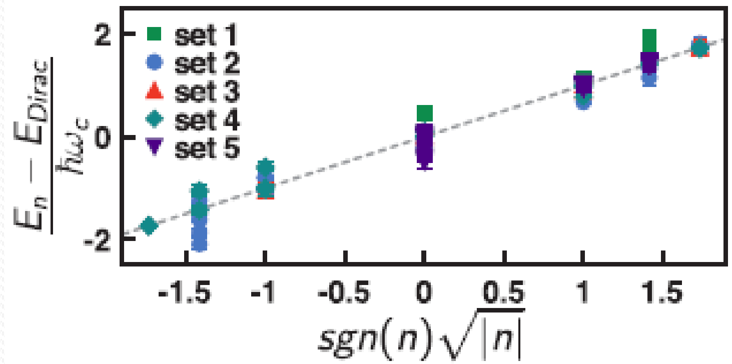
Pseudo–Magnetic Fields in Graphene Nanobubble







Linear Fitting



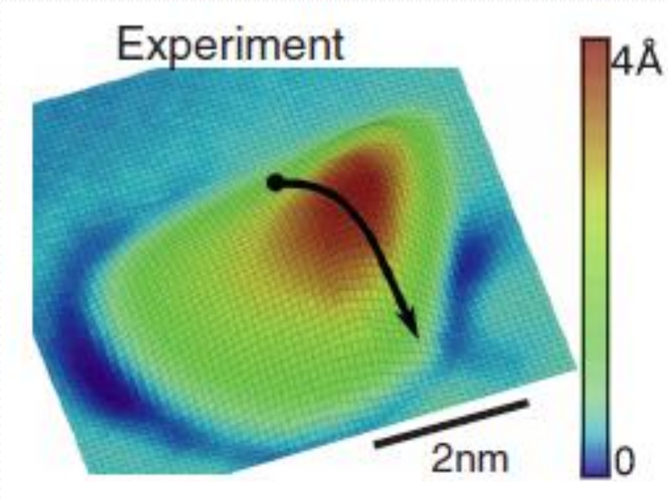
Graphene landau level

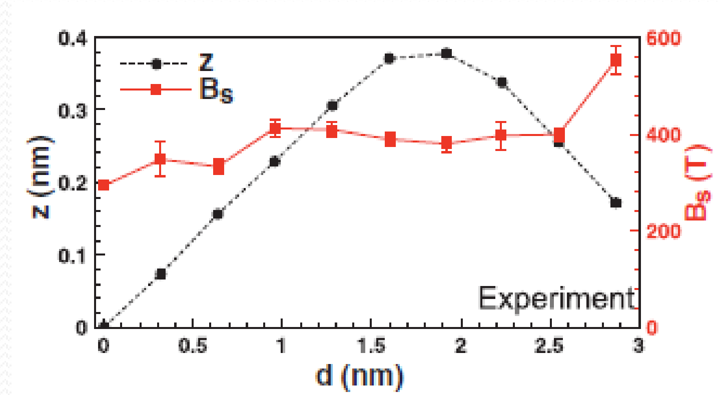
$$E_n = \mathrm{sgn}(n)\hbar\omega_c\sqrt{|n|} + E_{\mathrm{Dirac}},$$

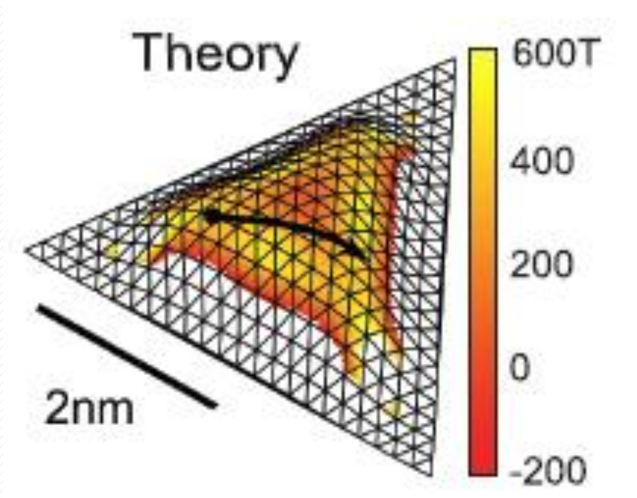
$$\omega_c = \sqrt{2e\hbar v_F^2 B_s}$$

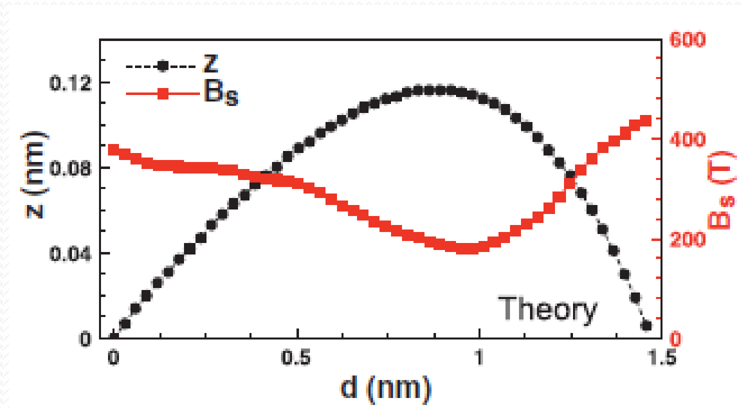
N. Levy, *et al.*
Science 329, 544 (2010)

Strain-Induced Pseudo–Magnetic Fields ?









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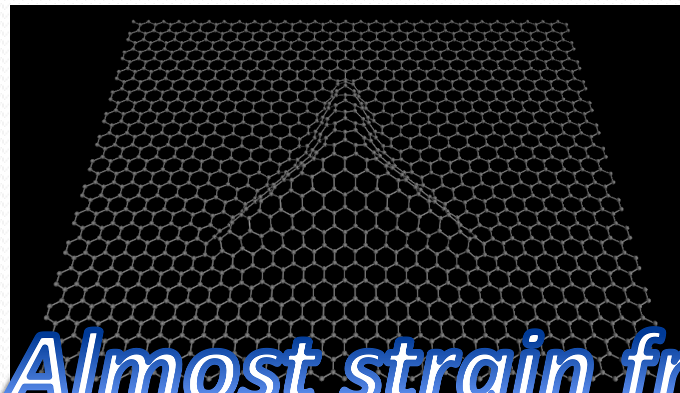
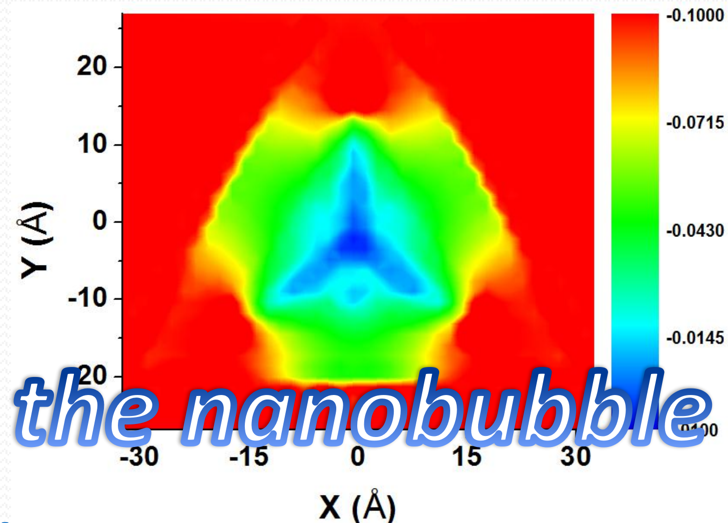
Is This Really the "Strain-Induced" Pseudo–Magnetic Field Effect ?

- **Strain effect ?**
- **Curvature effect ?**

Strain Map of 2D Graphene Nanobubble

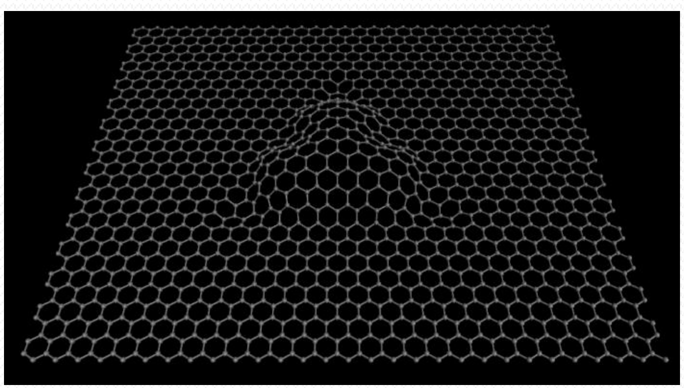
- Case one: fix z (10% strain)

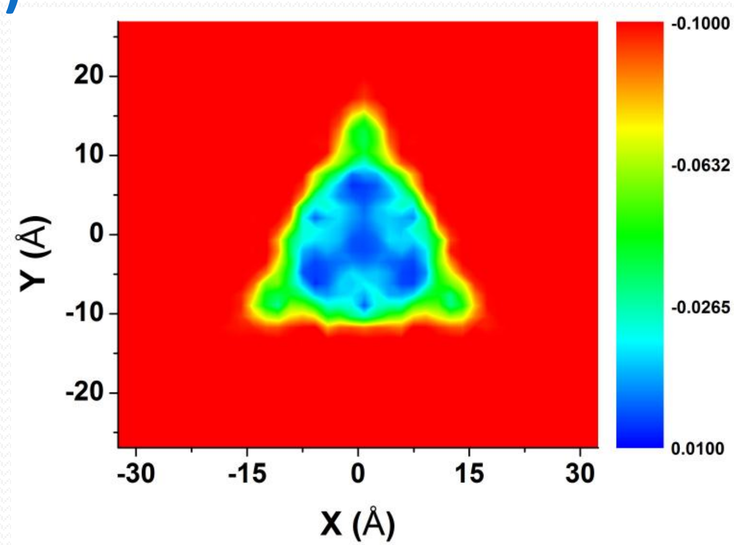




Almost strain free in the nanobubble

- Case two: relax all (10% strain)





1D Graphene Nanobubble