Nano-Kirigami and strain physics in 2D materials

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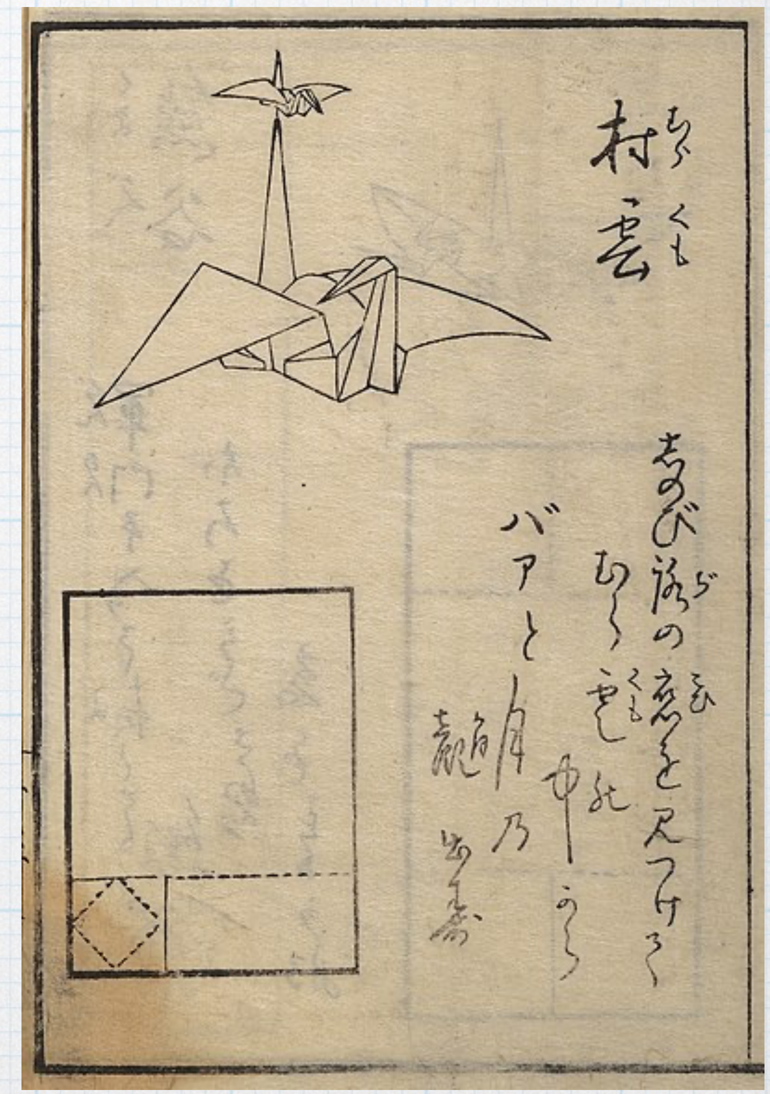
Origami (Paper folding)

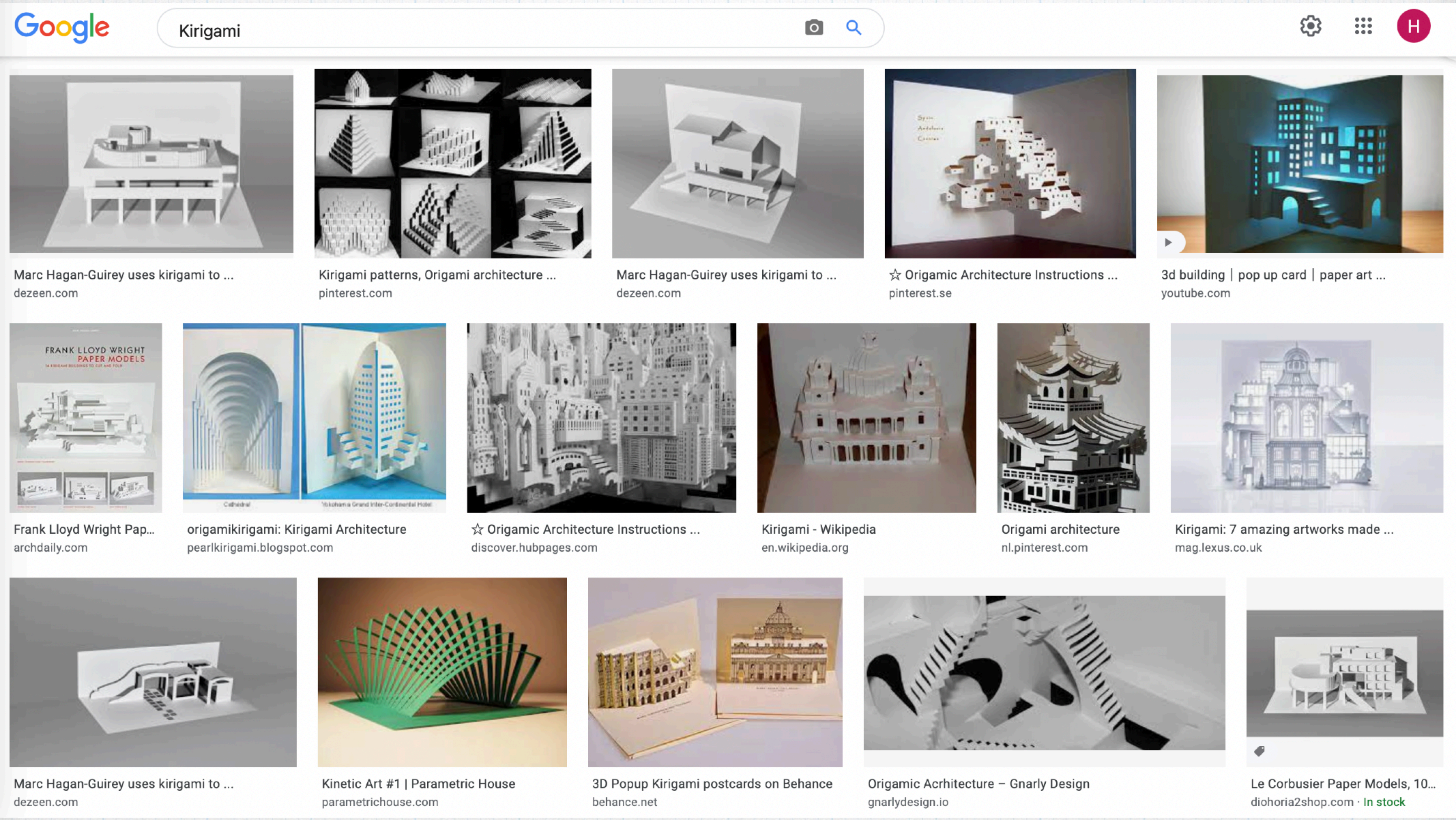
The word 'origami' consists of two Japanese characters - ori, which means 'bend' or 'fold' and kami, that is 'paper.'

Wikipedia



Wikipedia: The folding of two origami cranes linked together, from the first known book on origami, *Hiden senbazuru orikata*, published in Japan in 1797

Kirigami (cutting and folding)



Stretchable and Foldable Silicon Integrated Circuits [Science 320, 507 (2008)]

Aim: personal health monitors and other biomedical devices, that require extreme mechanical deformations

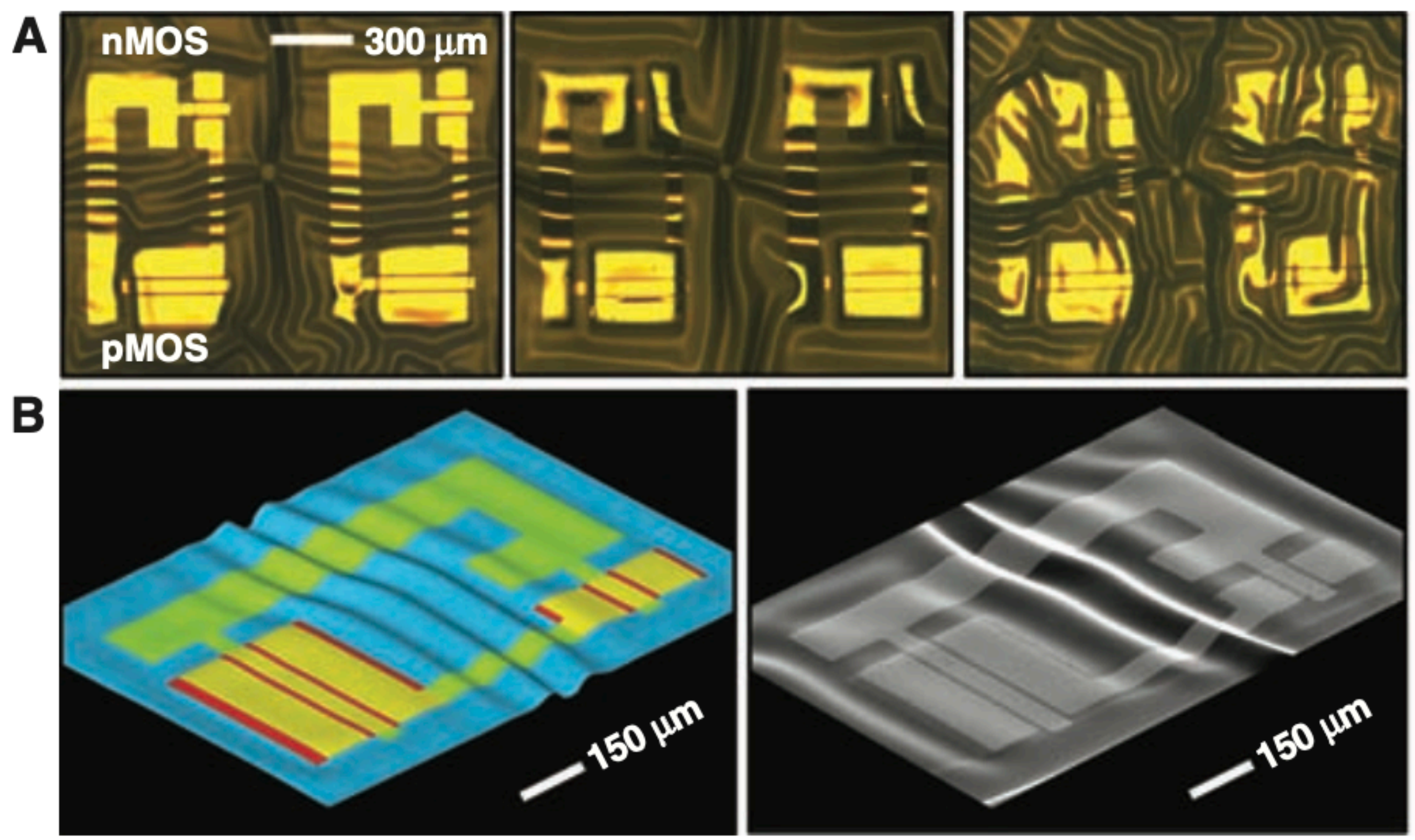
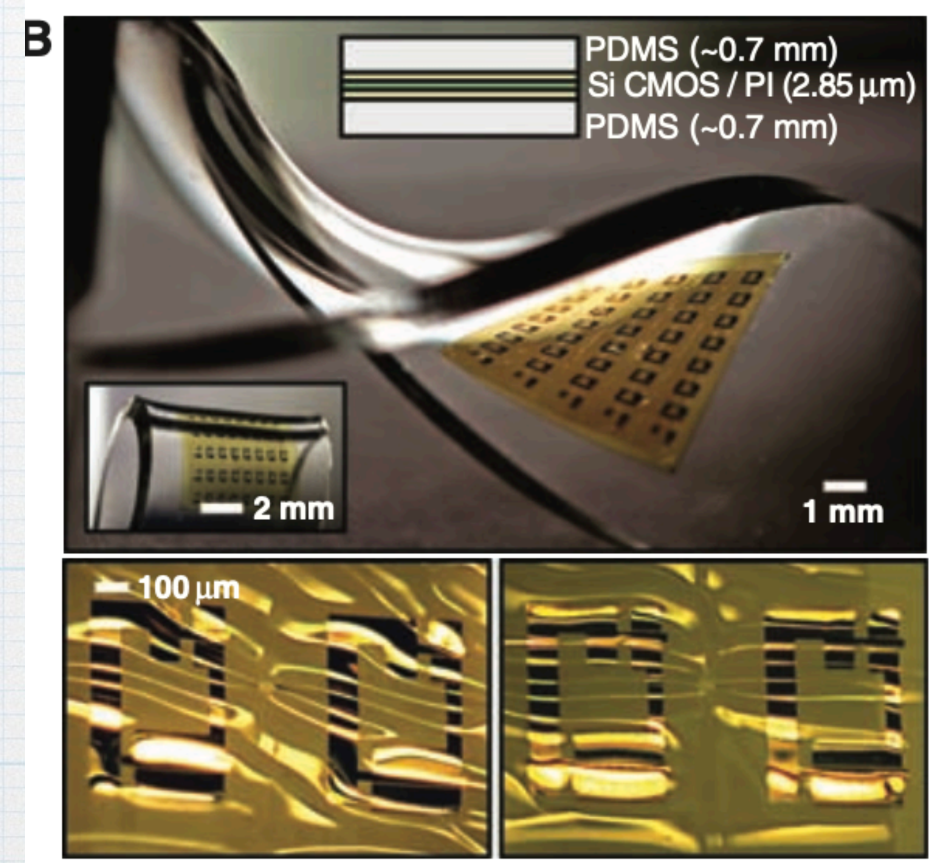
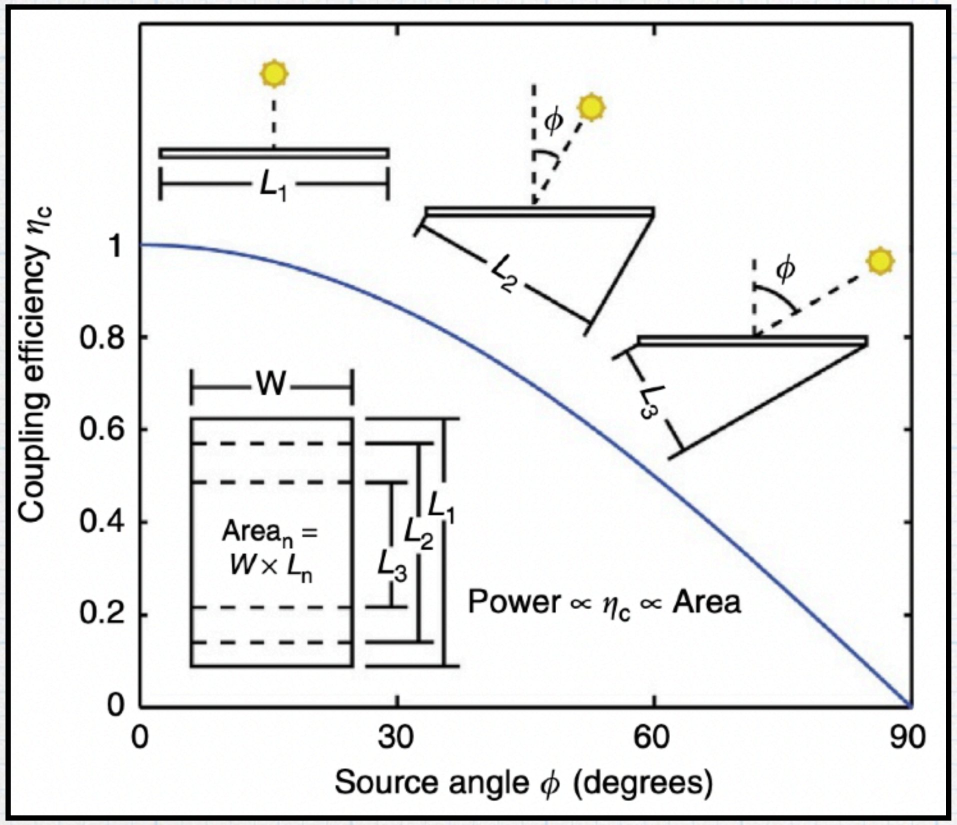
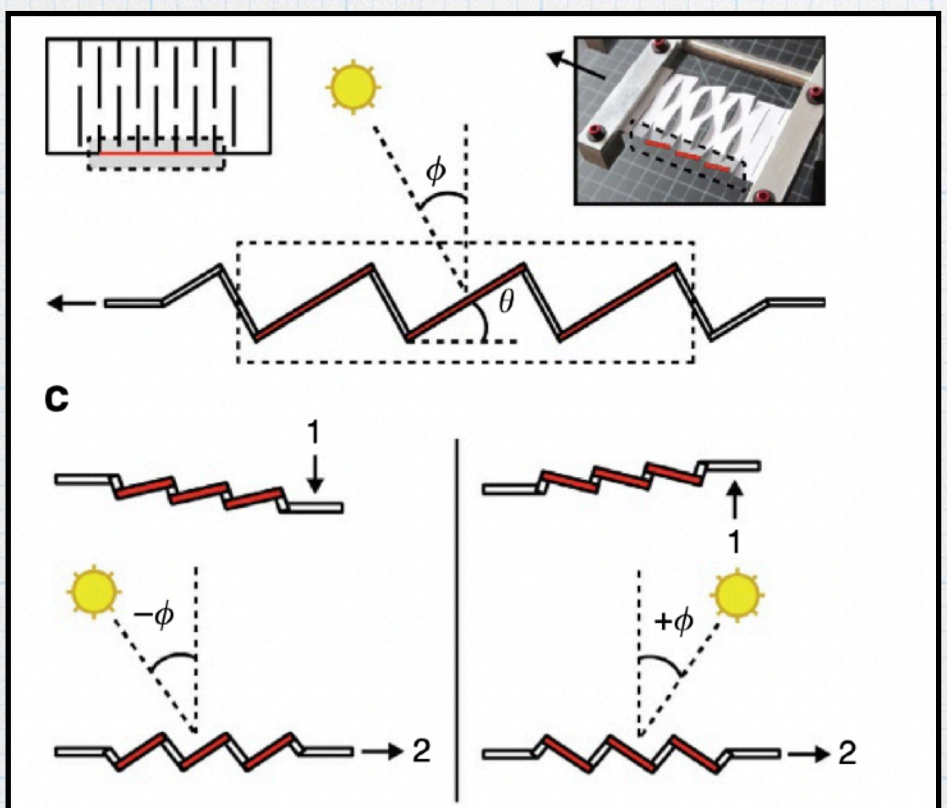


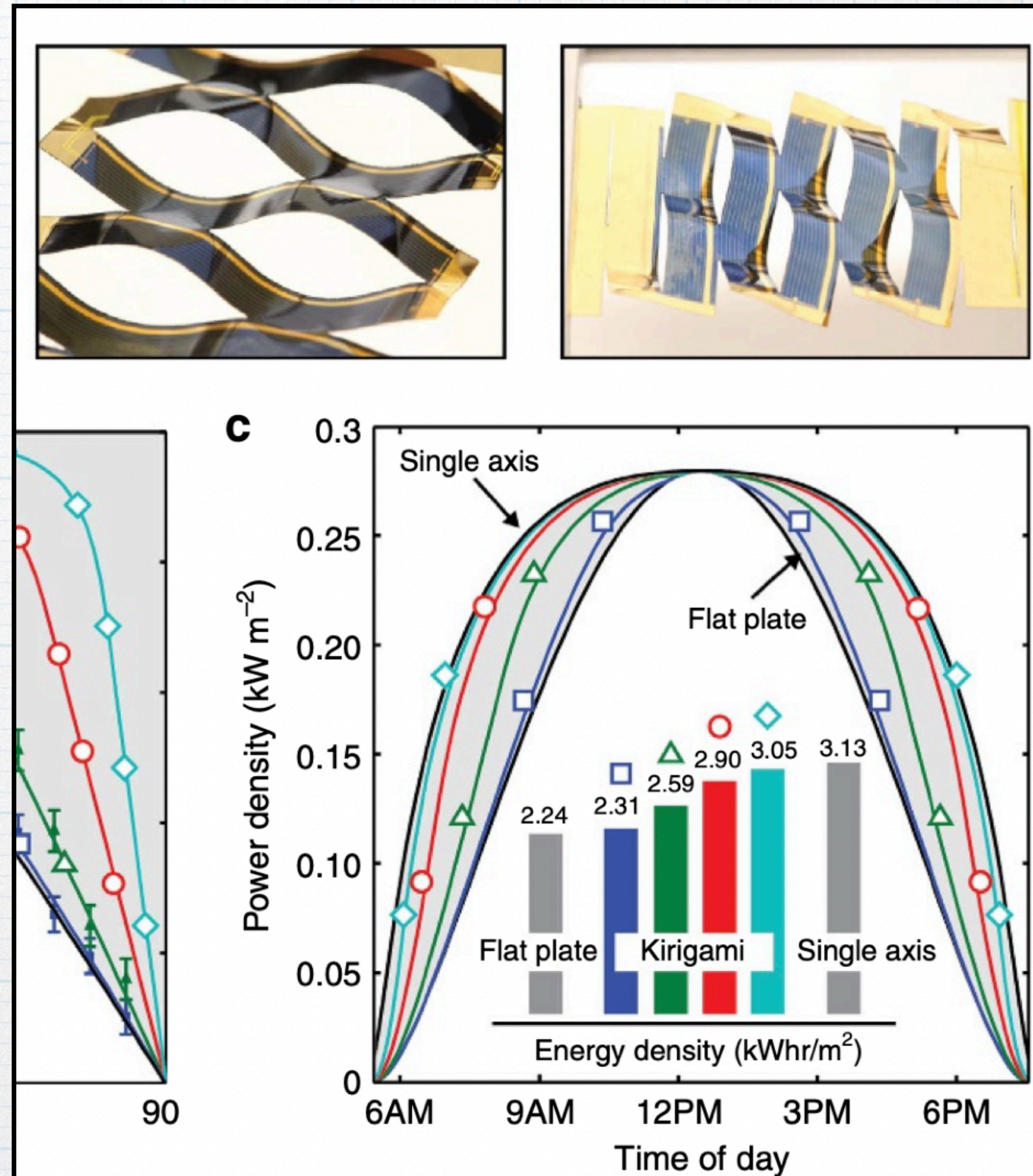
Fig. 2. (**A**) Wavy Si-CMOS inverters on PDMS, formed with various levels of prestrain. (left, ε_{pre} = 2.7%; center, ε_{pre} = 3.9%; right, ε_{pre} = 5.7%.) (**B**) Structural configuration determined by full 3D FEM of a system formed with ε_{pre} = 3.9% (left) and perspective scanning electron micrograph of a sample fabricated with a similar condition (right). (**C**) Optical images of wavy Si-CMOS



Dynamic kirigami structures for integrated solar tracking (GaAs Paper)



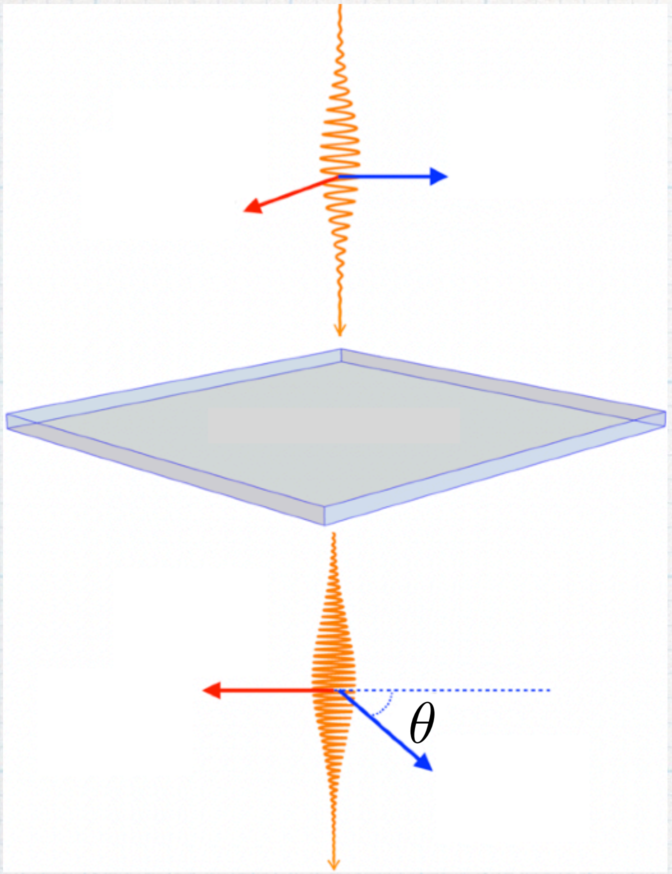


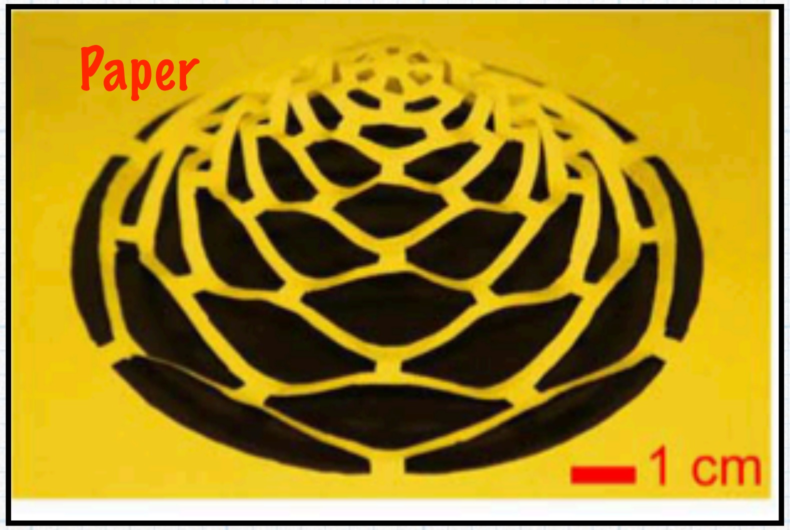


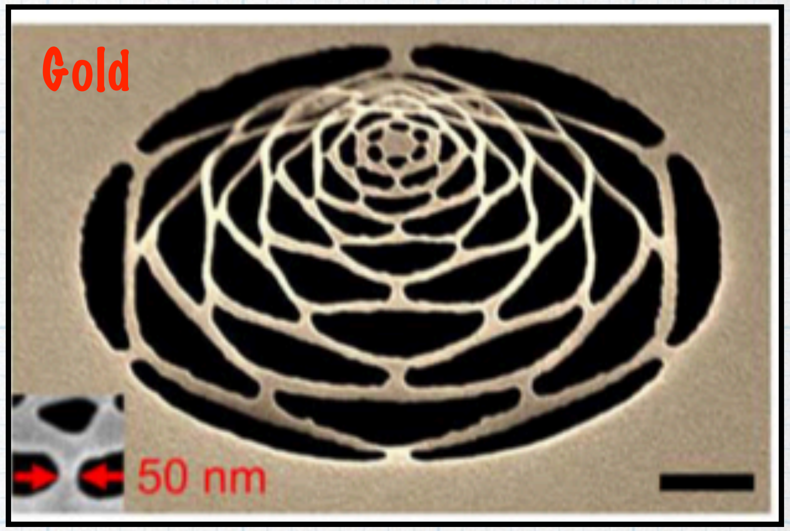
Nature Communications 6, 8092 (2015)

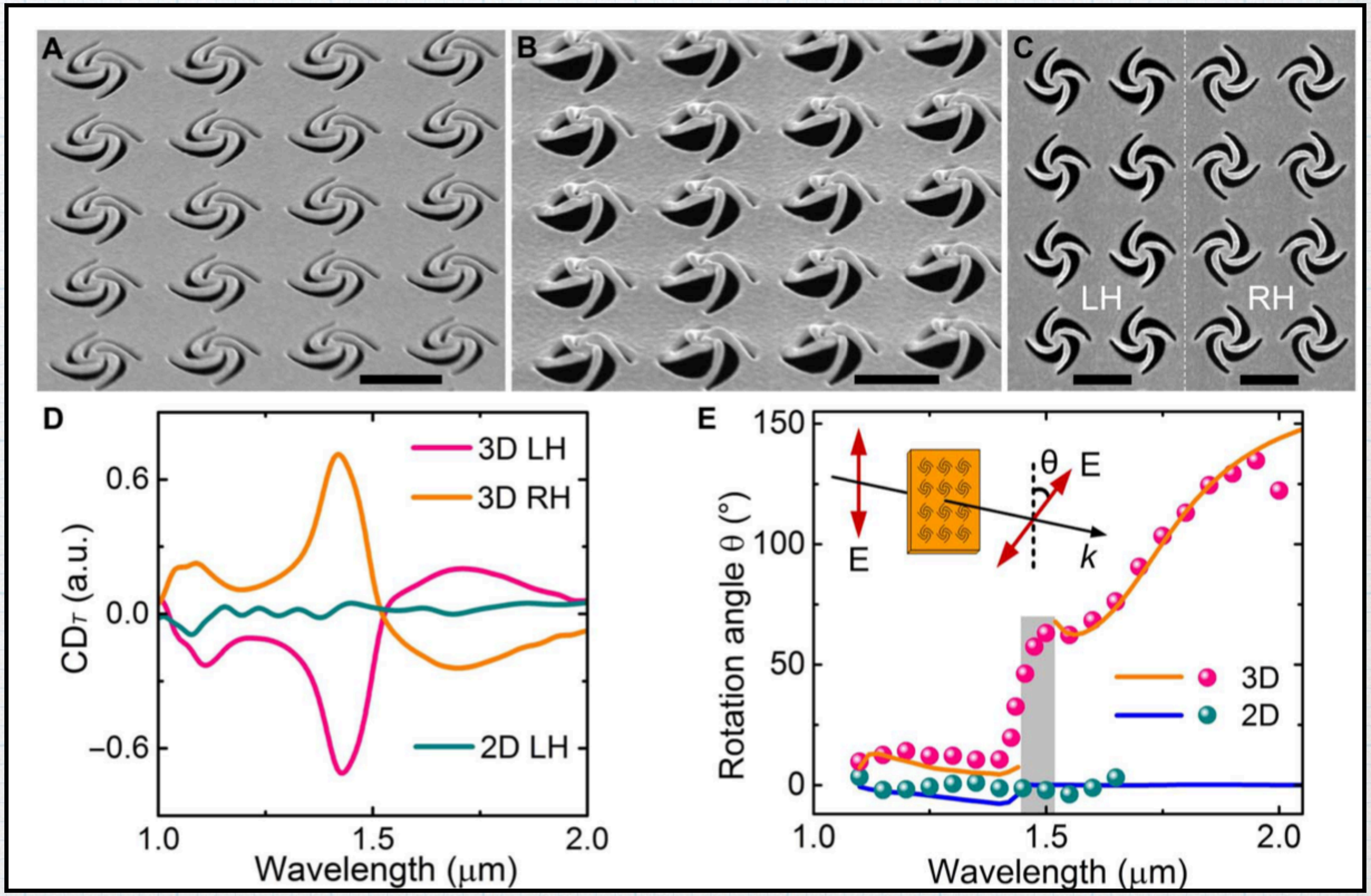
Nano-kirigami with giant optical chirality

Sci Adv 4 (7), eaat4436. (2018).







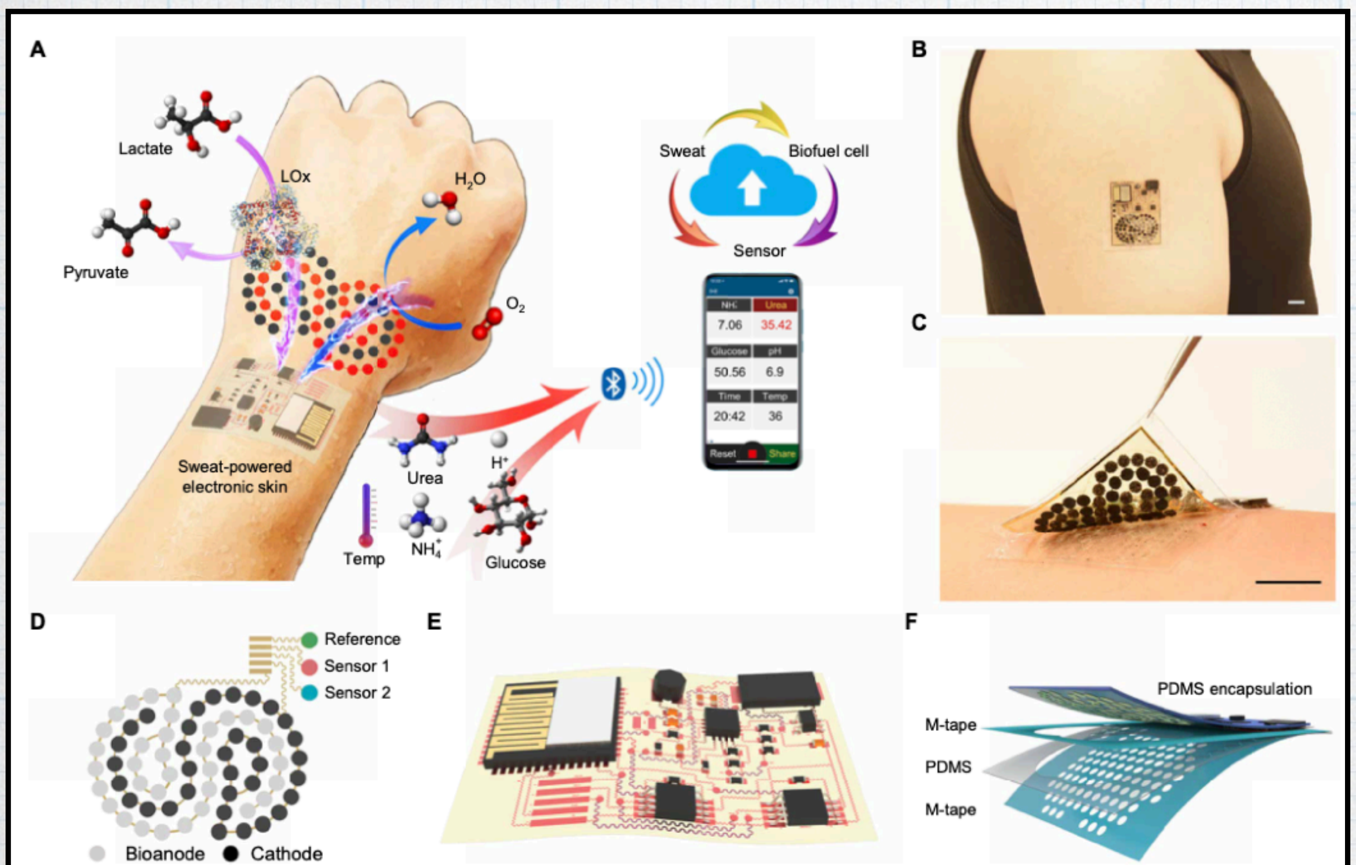


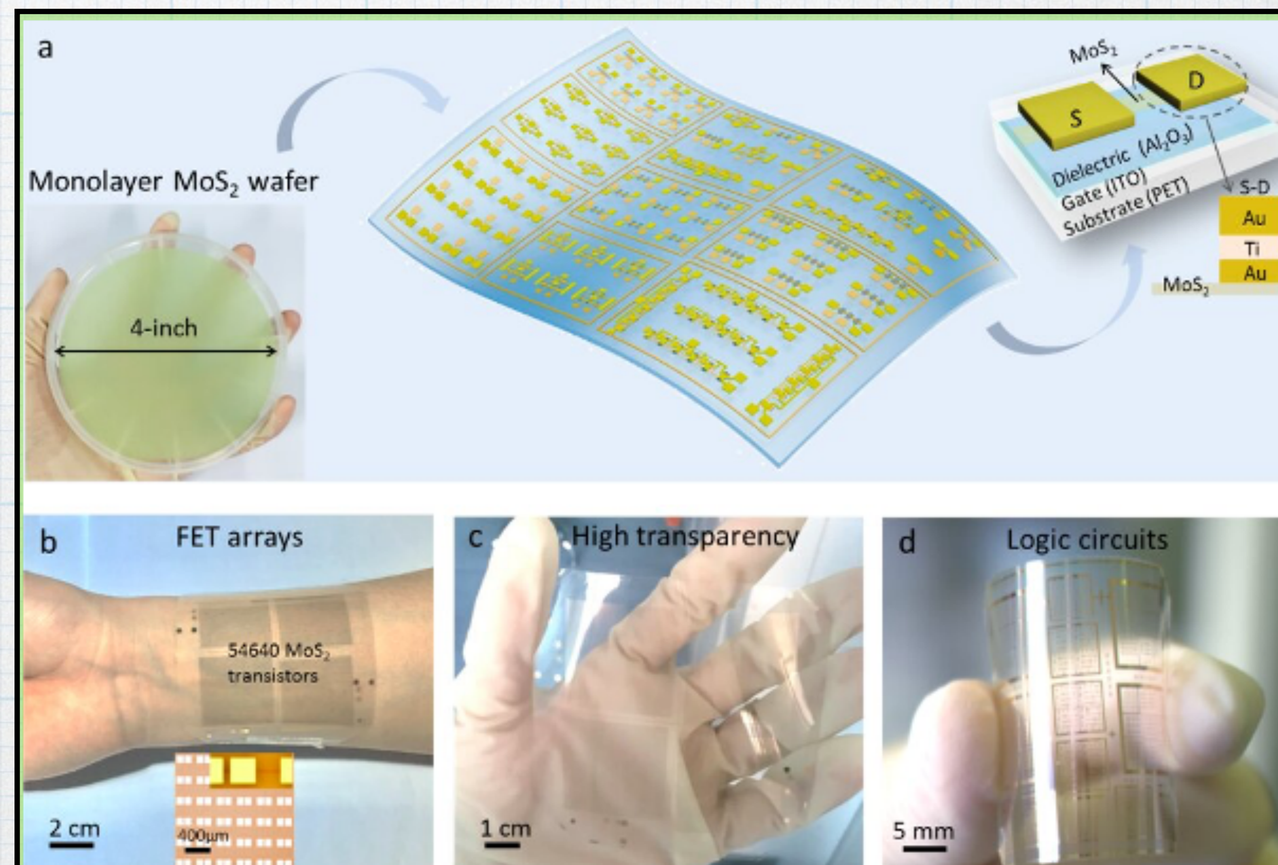
Circular Dichroism

$$CD = \frac{I_{\mathrm{LH}} - I_{\mathrm{RH}}}{I_{\mathrm{LH}} + I_{\mathrm{RH}}}$$

Wearable technology: flexible transparent electronic device

—Electronic skins
—human-machine interfaces
—Soft robotics
—Health monitoring
—entertainment technology
—Harvesting solar energy



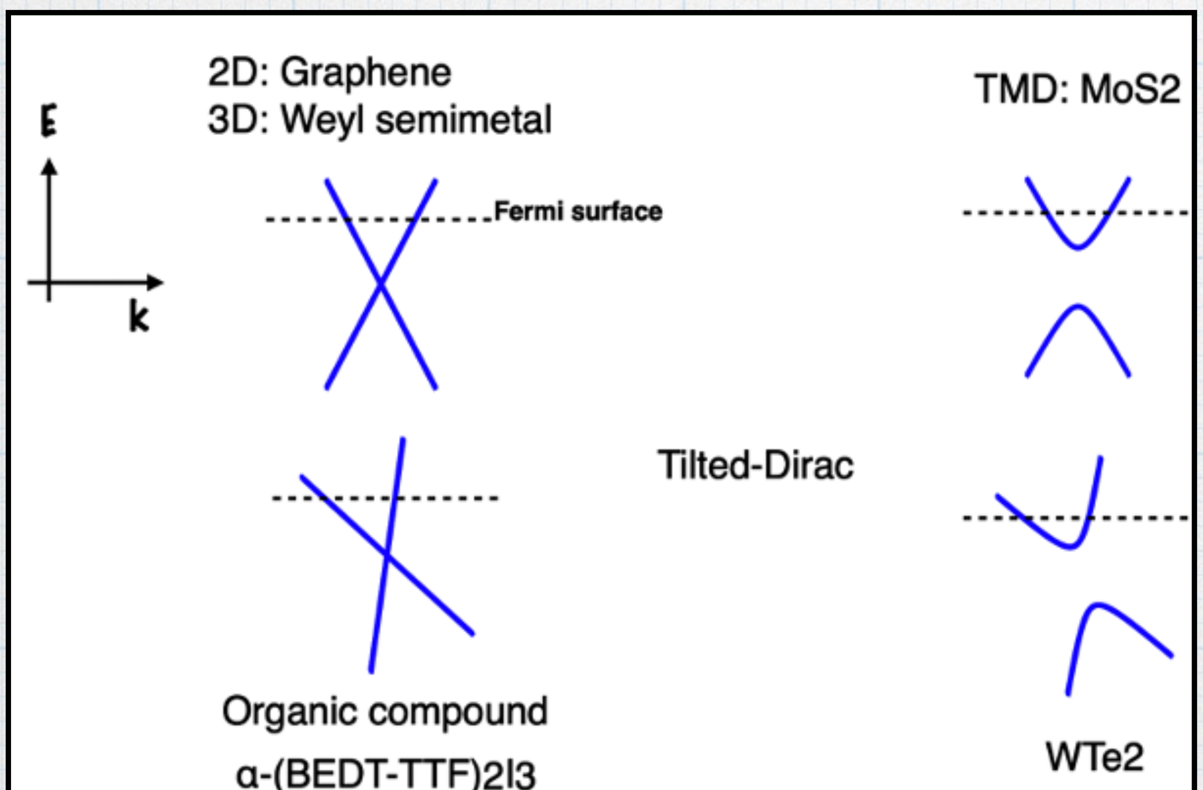


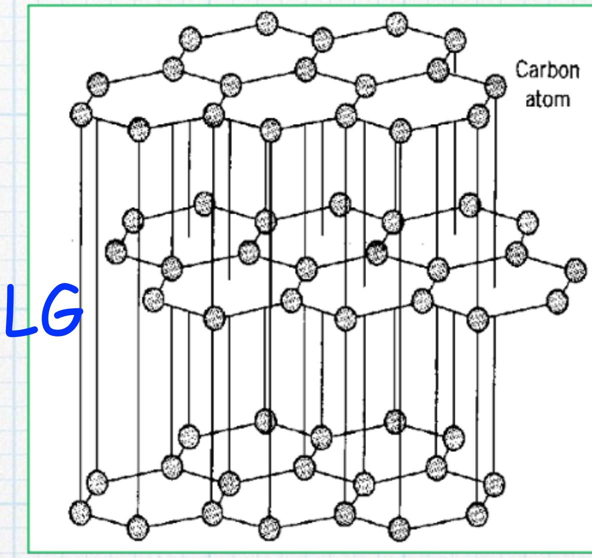
Yu et al., Sci. Robot. 5, eaaz7946 (2020)

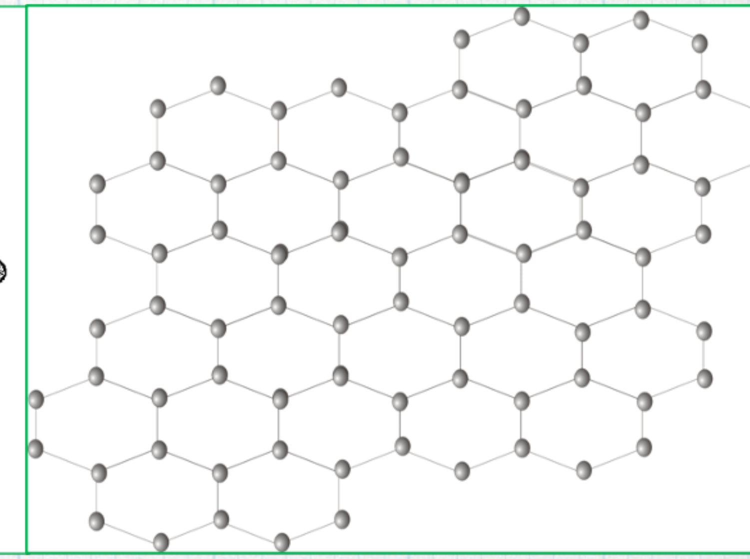
Nature Electronics 3, 711 (2020)

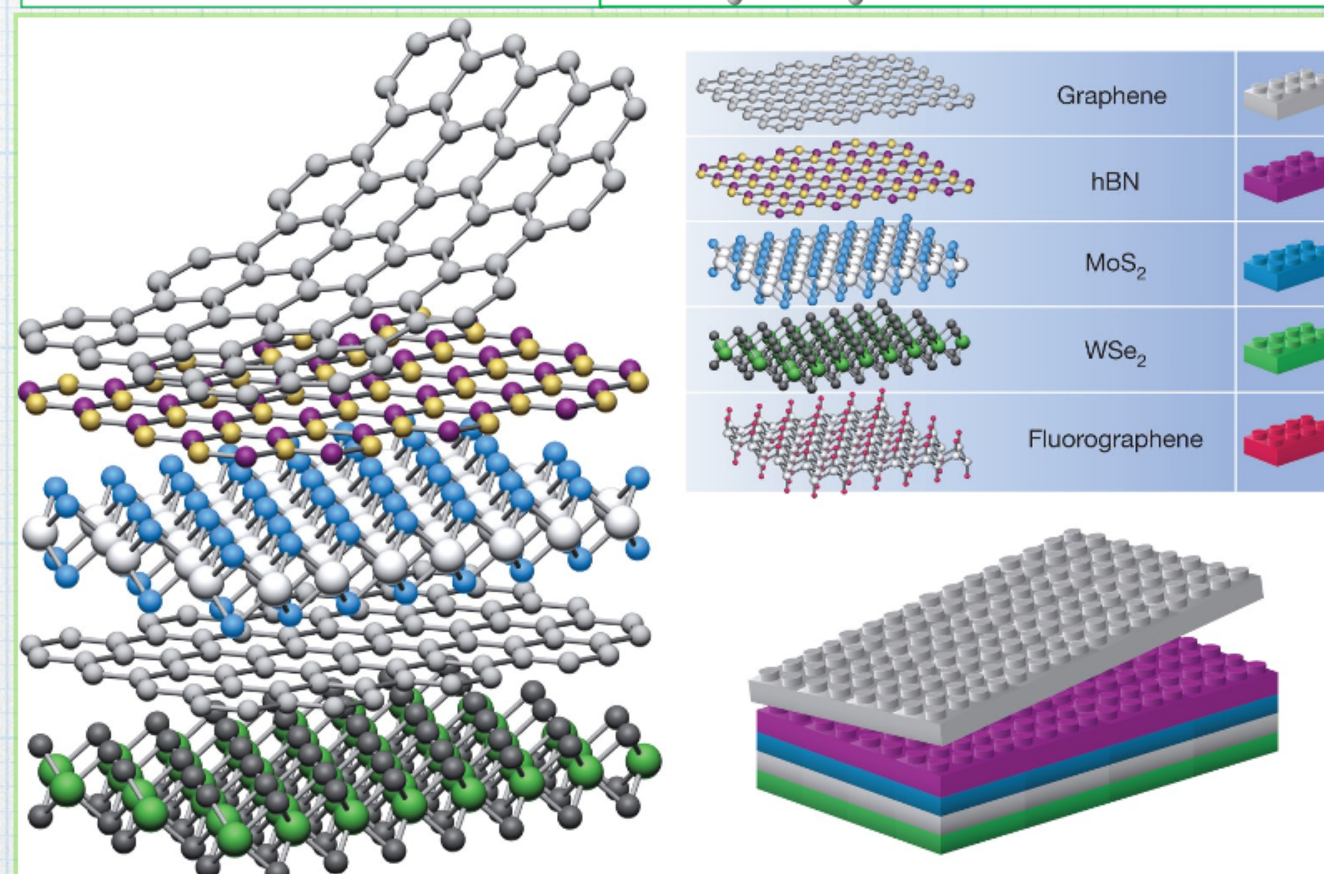
Van der Waals Layered Materials

—Easy to incorporate in nanothecnology,
—Extraordinary mechanical properties: Y~1TPA
—Universal properties: Dirac materials,
—High performance transport,
—Exotic optical properties,
—Strong many-body correlation: Twisted BLG
—Nontrivial topology: QSH in WTe2









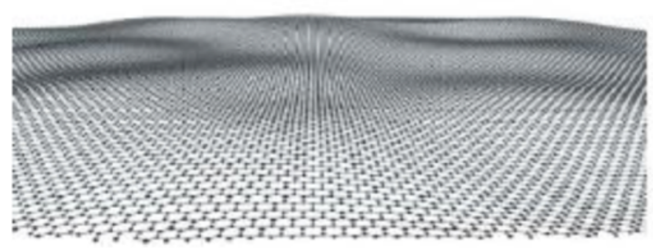
Nature 499, 419 (2013)

LETTERS

The structure of suspended graphene sheets

Jannik C. Meyer[1], A. K. Geim[2], M. I. Katsnelson[3], K. S. Novoselov[2], T. J. Booth[2] & S. Roth[1]

Scale bar, 500 nm



Ripple in Graphene

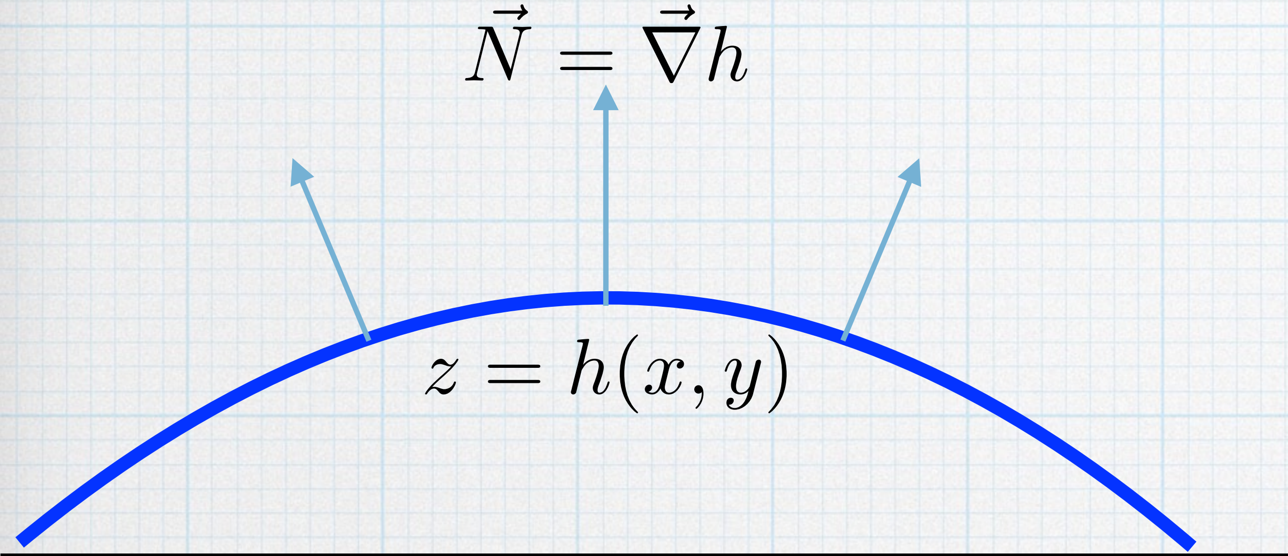
Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene

Changgu Lee,[1,2] Xiaoding Wei,[1] Jeffrey W. Kysar,[1,3] James Hone[1,2,4]*

We measured the elastic properties and intrinsic breaking strength of free-standing monolayer graphene membranes by nanoindentation in an atomic force microscope. The force-displacement behavior is interpreted within a framework of nonlinear elastic stress-strain response, and yields second- and third-order elastic stiffnesses of 340 newtons per meter ($N\ m^{-1}$) and –690 $N\ m^{-1}$, respectively. The breaking strength is 42 $N\ m^{-1}$ and represents the intrinsic strength of a defect-free sheet. These quantities correspond to a Young's modulus of E = 1.0 terapascals, third-order elastic stiffness of D = –2.0 terapascals, and intrinsic strength of σ_{int} = 130 gigapascals for bulk graphite. These experiments establish graphene as the strongest material ever measured, and show that atomically perfect nanoscale materials can be mechanically tested to deformations well beyond the linear regime.

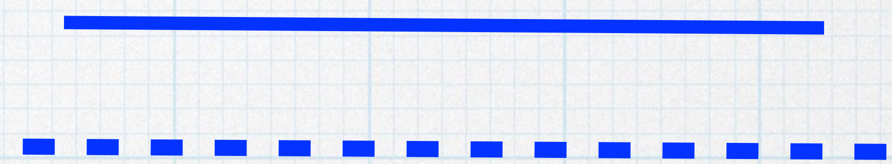
Graphene as a 2D elastic membrane

Bending energy



$$F_b \approx \frac{1}{2}\kappa \int dxdy(\vec{\nabla} \cdot \vec{N})^2$$
$$= \frac{1}{2}\kappa \int dxdy(\nabla^2 h)^2$$

Stretching energy



$$F_t \approx Y \int dxdy\{\sqrt{1 + |\nabla h|^2} - 1\}$$
$$\approx \frac{1}{2} Y \int dxdy |\nabla h|^2$$

1 TPa 0.1 nm

$$Y_{2D} = Y_{3D} t \sim 10^{12}\mathrm{N/m^2} \times 10^{-10}\mathrm{m} \sim 100\mathrm{N/m}$$

Föppl-von Kármán number vK

$$vK = \frac{Y_{2D} L^2}{\kappa} \qquad \kappa \sim Y_{2D} t^2 / 10$$

Y_2D: two-dimensional Young's modulus ([Y_2D]=N/m)

kappa: bending rigidity ([kappa]=J)

L: sheet side length

t: sheet thickness

$$vK \sim 10(L/t)^2$$

$L \sim 100nm,$

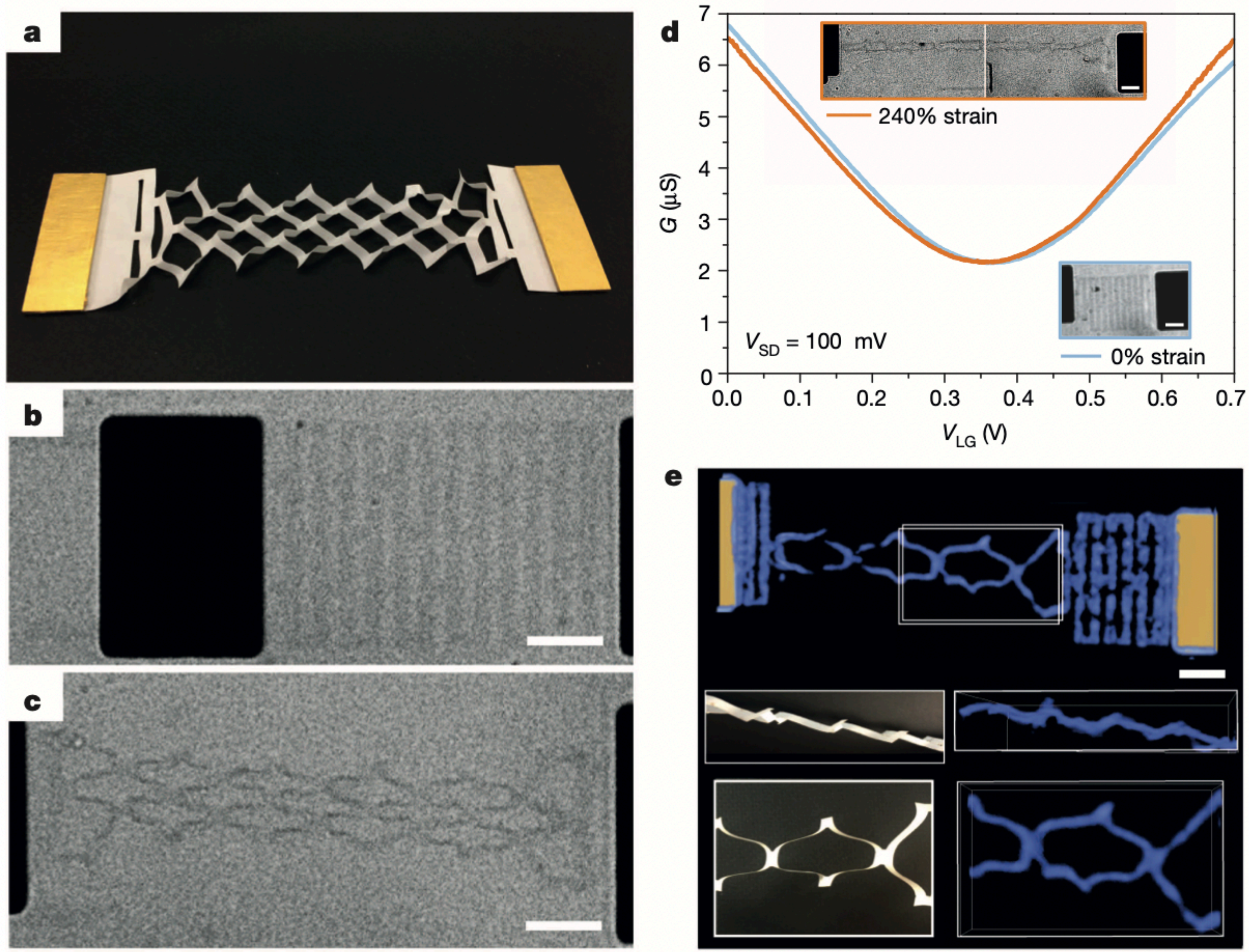
paper: $\quad t \sim 0.1mm \to vK \sim 10^{-5}$

graphene: $t \sim 0.1nm \to vK \sim 10^{7}$

For large vK we can easily bend the sheet without energy cost for stretching.

Graphene kirigami

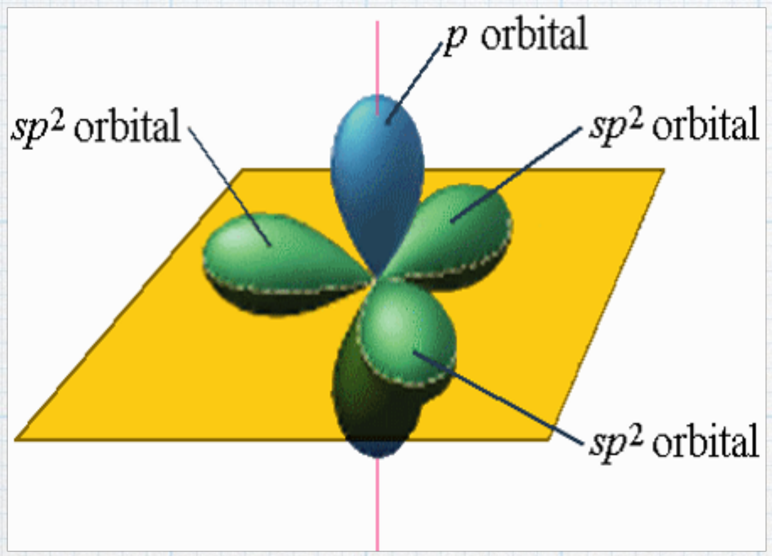
Nature 524, 204–207 (2015)

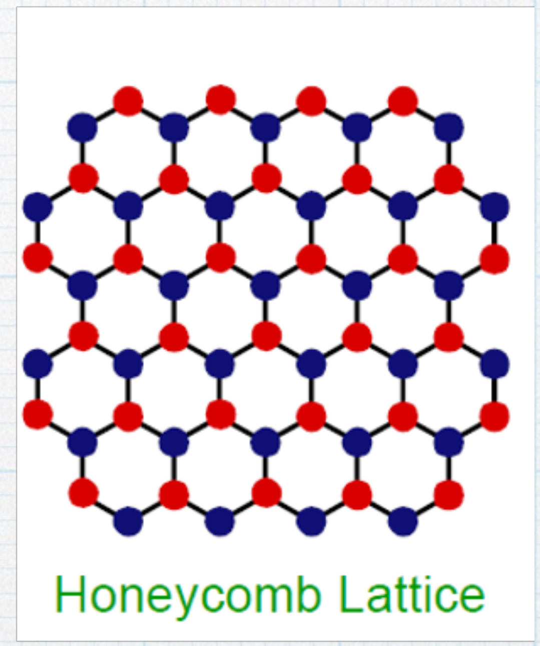


Graphene as an electronic membrane

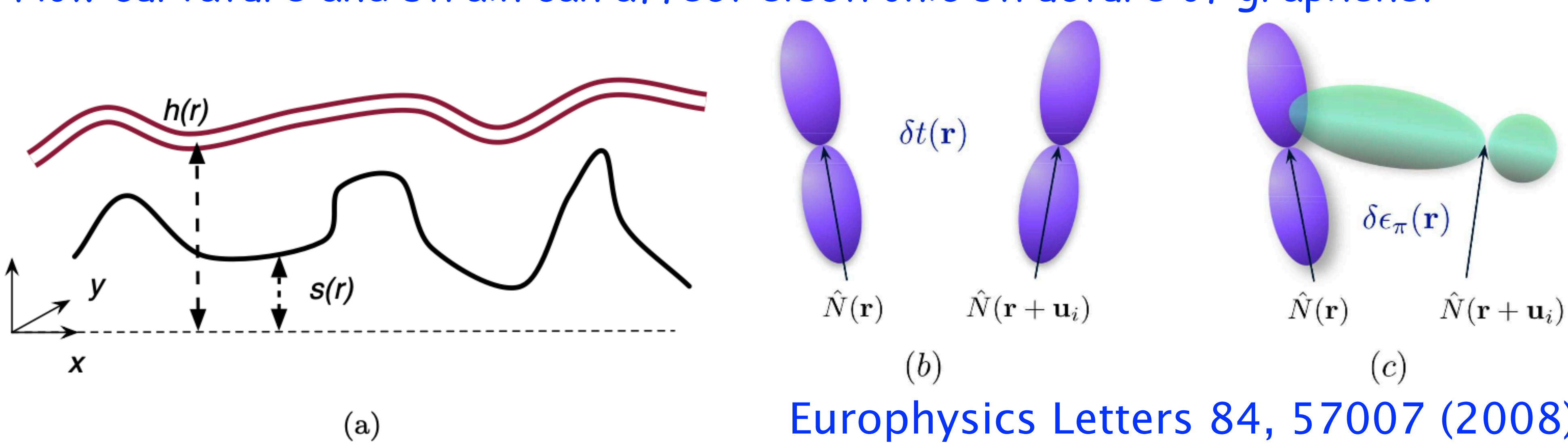
$$\text{Carbon atom} \quad : 1s^2 2s^2 2p^2$$

$$: ({\color{red}two})1s^2 + ({\color{red}three})sp^2 + ({\color{red}one})2p_z$$





How curvature and strain can affect electronic structure of graphene?



Europhysics Letters 84, 57007 (2008)

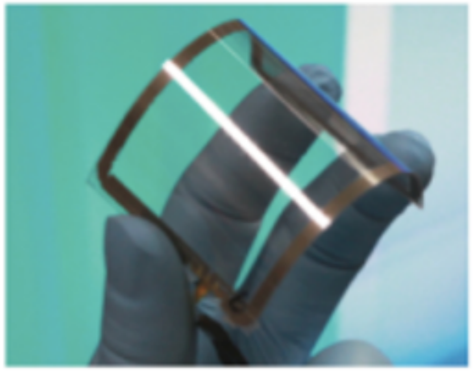
Flexible and transparent devices

nature nanotechnology

LETTERS

PUBLISHED ONLINE: 20 JUNE 2010 | DOI: 10.1038/NNANO.2010.132

Roll-to-roll production of 30-inch graphene films for transparent electrodes



Extraordinary
Young's Modulus~1TPa

Highly flexible to
out-of-plane deformation

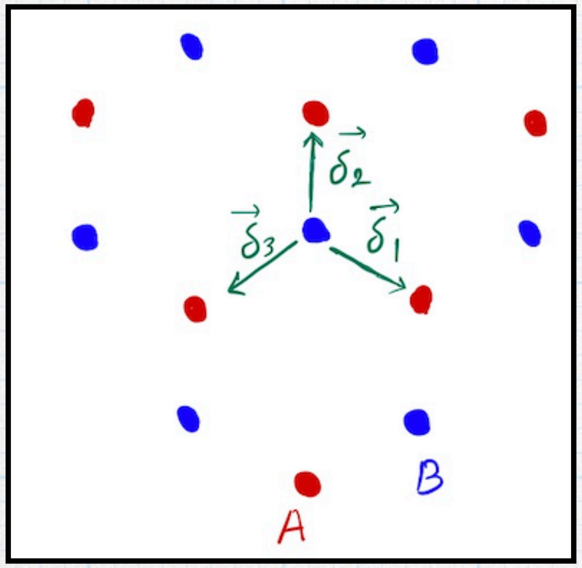
Ab initio: not practical for inhomogeneous strain

Curve space field theory: missing crystal symmetry

Tight-binding theory

K.p (invariant) method

Pseudo gauge field in hexagonal lattice



$$H = \sum_{R,\delta} t_\delta \, a^\dagger_R \, b_{R+\delta} + c.c.$$

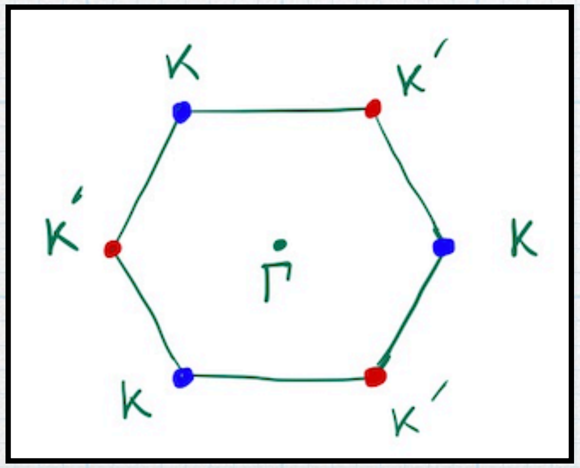
$$a_R = \frac{1}{\sqrt{N}} \sum_k e^{ik\cdot R} a_k$$

$$b_R = \frac{1}{\sqrt{N}} \sum_k e^{ik\cdot R} b_k$$

$$H = \sum_k (a^\dagger_k \ b_k)\, \hat H_k \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

$$\hat H_k = \begin{pmatrix} 0 & f_k \\ f^*_k & 0 \end{pmatrix}$$

$$f_k = \sum_\delta t_\delta \, e^{-ik\cdot\delta}$$



No strain: $t_\delta = t_0 \xrightarrow[\vec k = \vec K + q]{q \ll K} f_q \sim t_0 (q_x - i q_y)$

$\hat H \sim \vec\sigma \cdot \vec q$ $\qquad \hat\sigma_x = \tau \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \hat\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

Dirac model

$$\hat H \sim \vec\sigma \cdot (\vec q + \tau e \vec A)$$

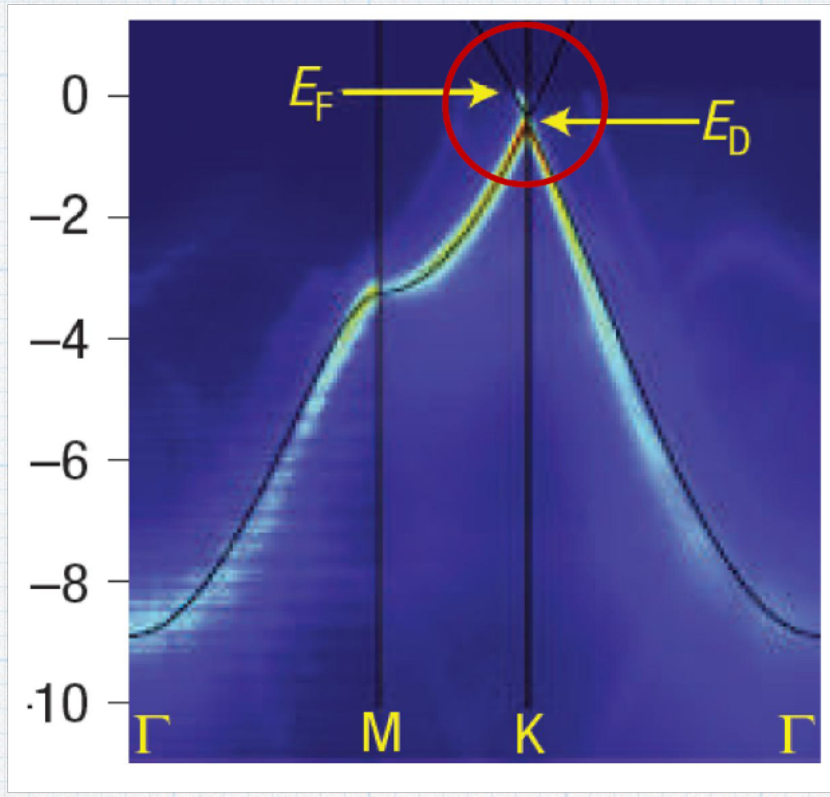
$\tau = +1 \longrightarrow K$ valley

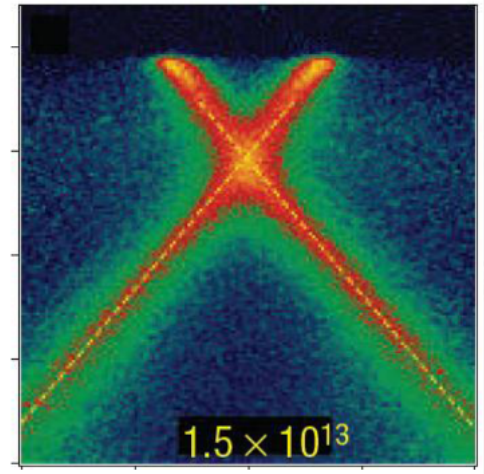
$\tau = -1 \longrightarrow K'$ valley

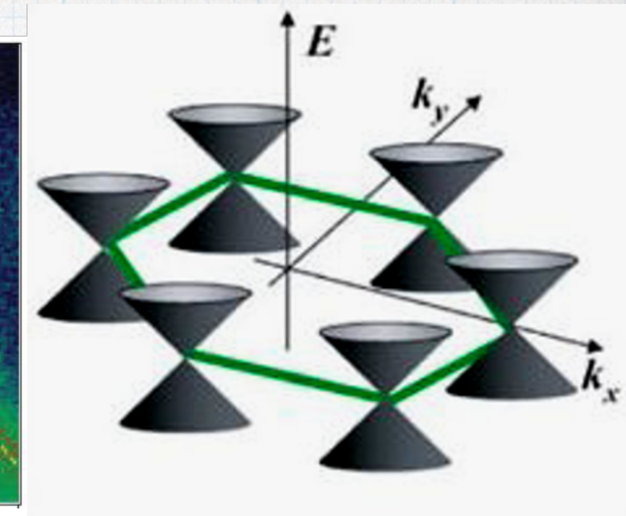
Pseudo gauge field:

$$A_x = t_{\delta_2} - \frac{t_{\delta_1} + t_{\delta_2}}{2}, \quad A_y = \frac{\sqrt{3}}{2}(t_{\delta_1} - t_{\delta_3})$$

Angle-resolved photoelectron spectroscopy (ARPES)





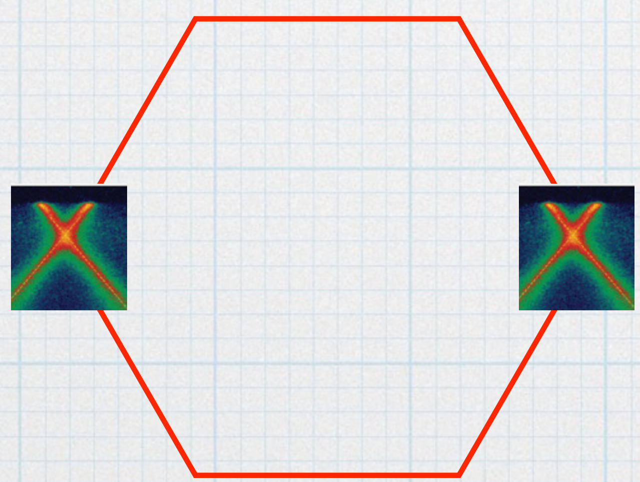


$$\mathcal{H} = \hbar v_{\mathrm{F}}(\tau q_x \sigma_x + q_y \sigma_y)$$

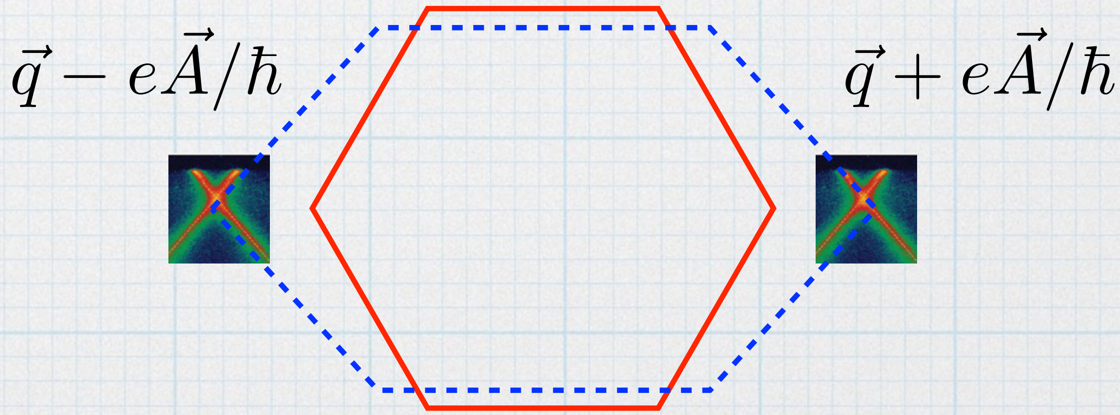
$$v_{\mathrm{F}} = \frac{3ta_0}{2\hbar} \approx 10^6 \frac{m}{s} \approx \frac{c}{300}$$

Each state is 4-fold degenerate, 2 for spin and 2 for valley

A.Bostwick, et al,2007, Nature Physics 3(1), 36.



Uniaxial strain

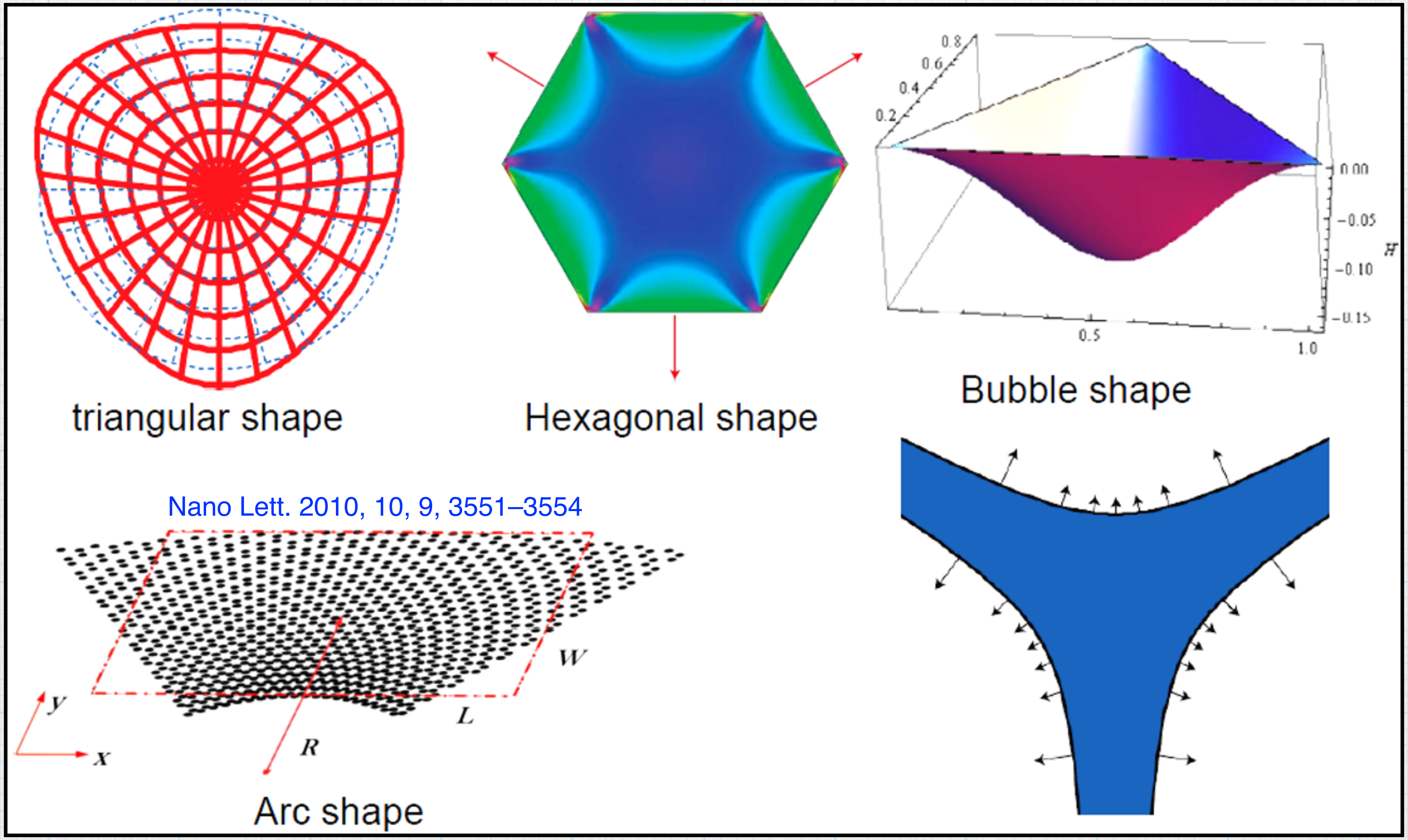


Uniform pseudomagnetic field

$$A_x = \beta(\hbar/ea)(u_{xx} - u_{yy})$$
$$A_y = \beta(\hbar/ea)(-2u_{xy})$$

$$\vec{B} = \vec{\nabla} \times \vec{A}$$

$$\beta = -\frac{\partial \ln t}{\partial \ln a}$$

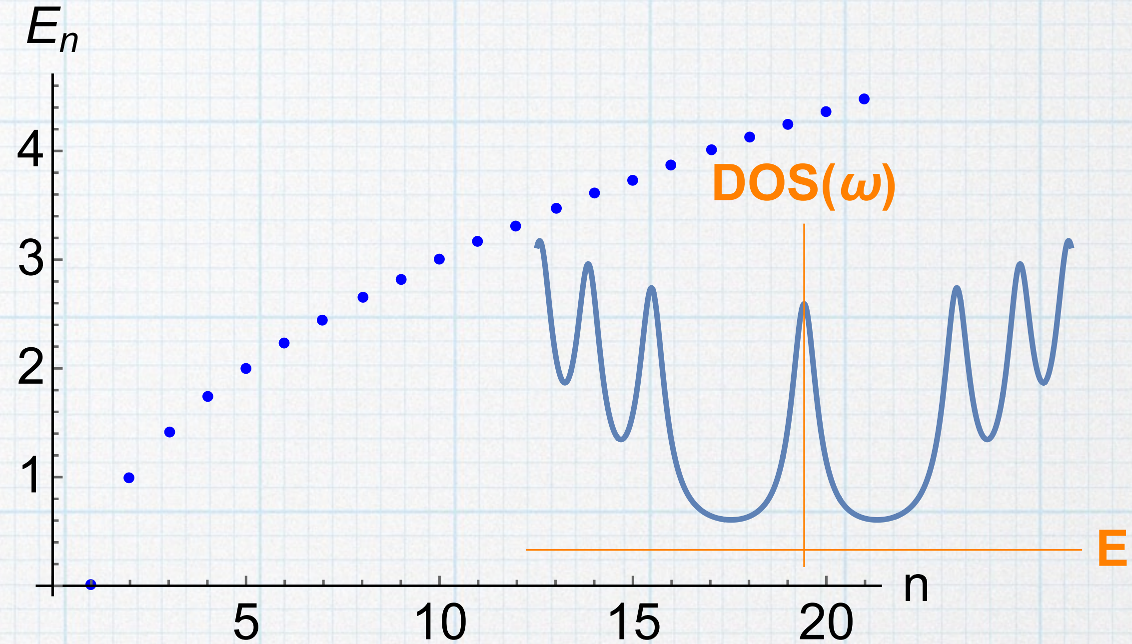


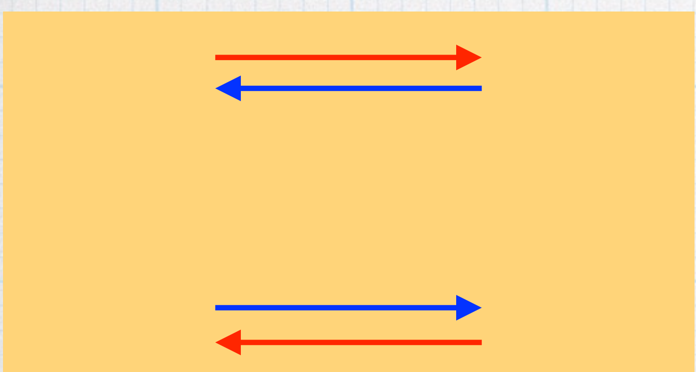
Guinea, F., Katsnelson, M. & Geim, A. Nature Phys 6, 30–33 (2010)

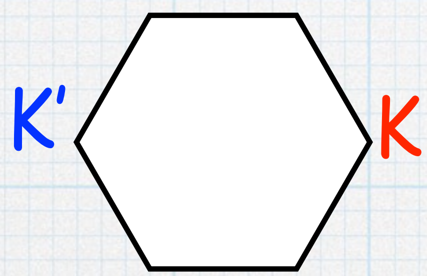
LDOS: Pseudo Landau Levels

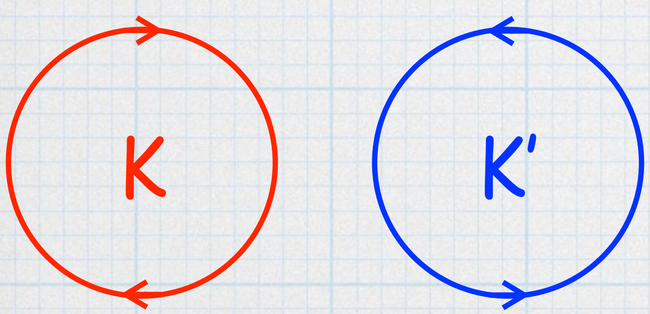
$$H = v_F \hat{\boldsymbol{\sigma}} \cdot (\mathbf{p} + e\mathbf{A}) \qquad \mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$$

$$E_n \approx 35\text{meV} \times \text{sign}(n) \times \sqrt{B[T]} \times \sqrt{|n|}$$

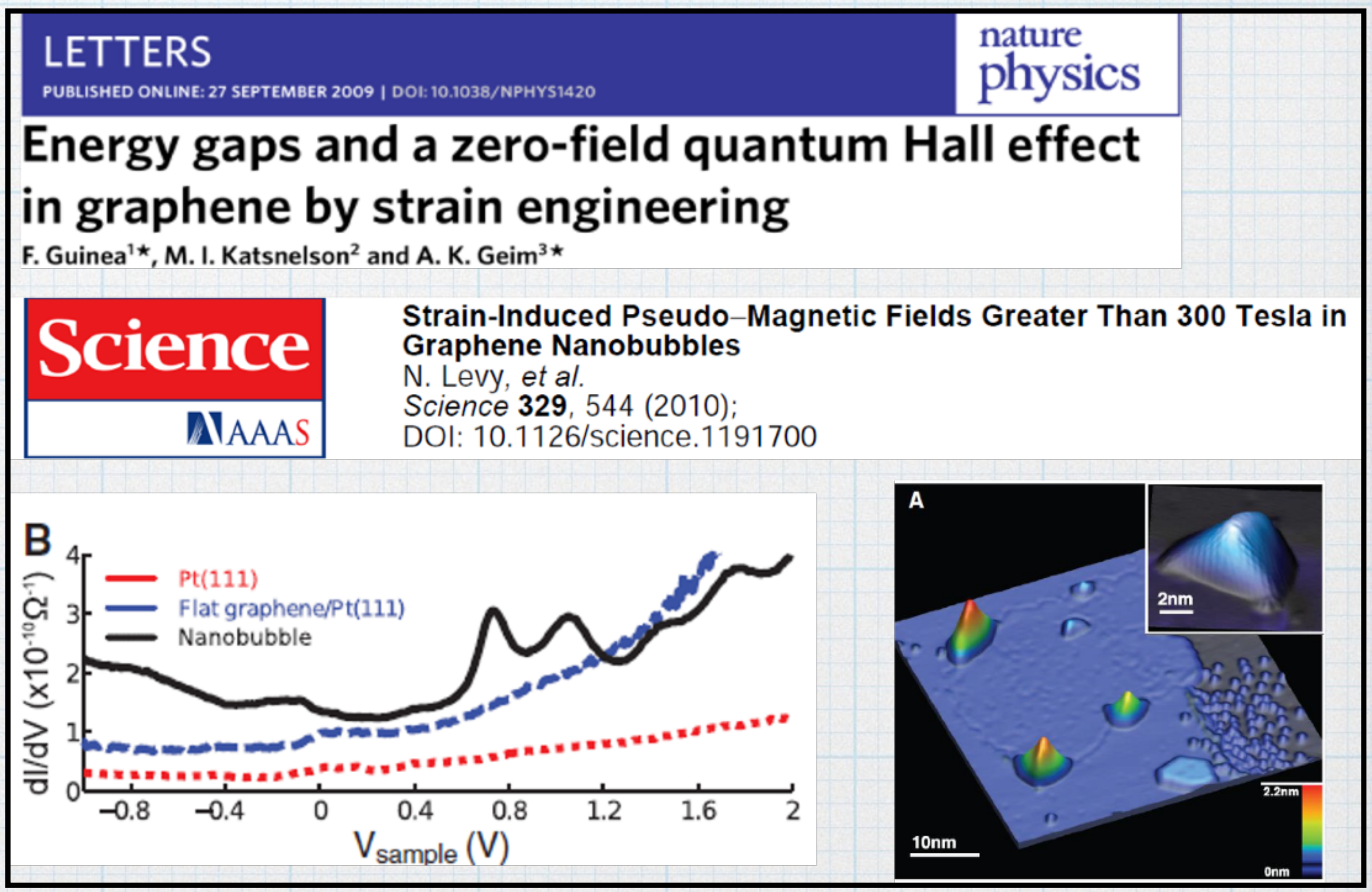




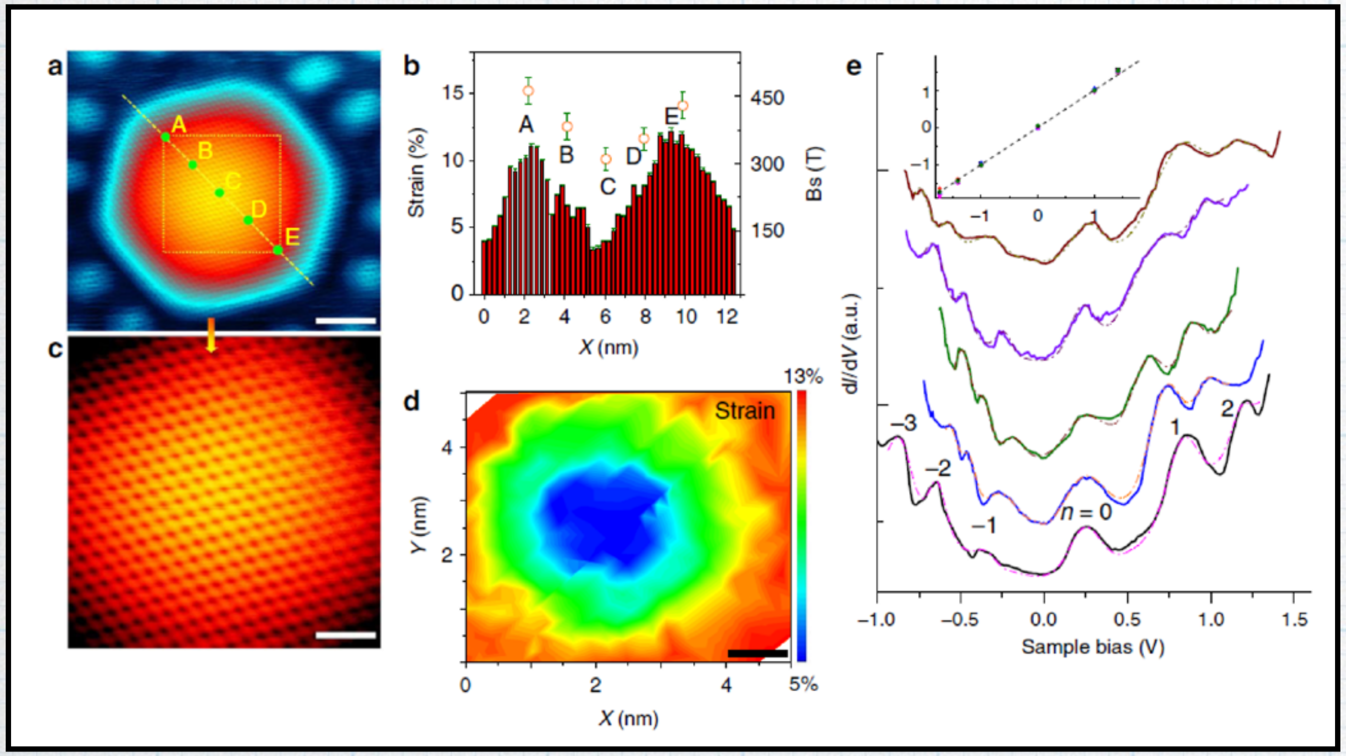




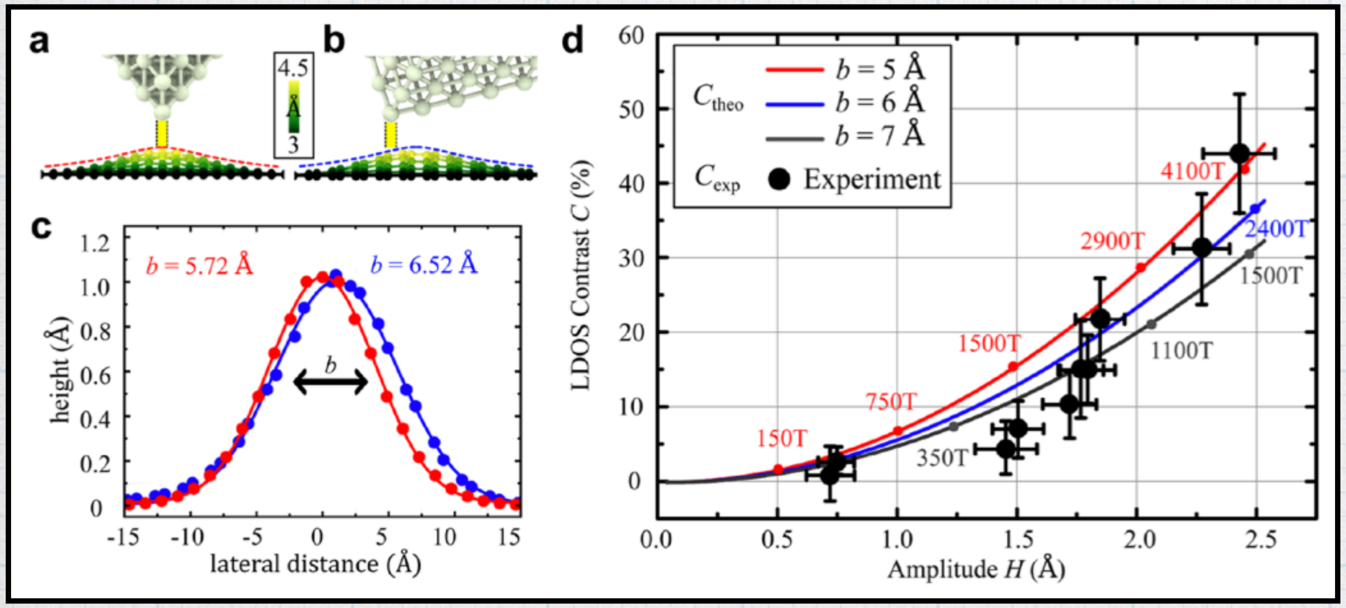
Quantum valley Hall effect



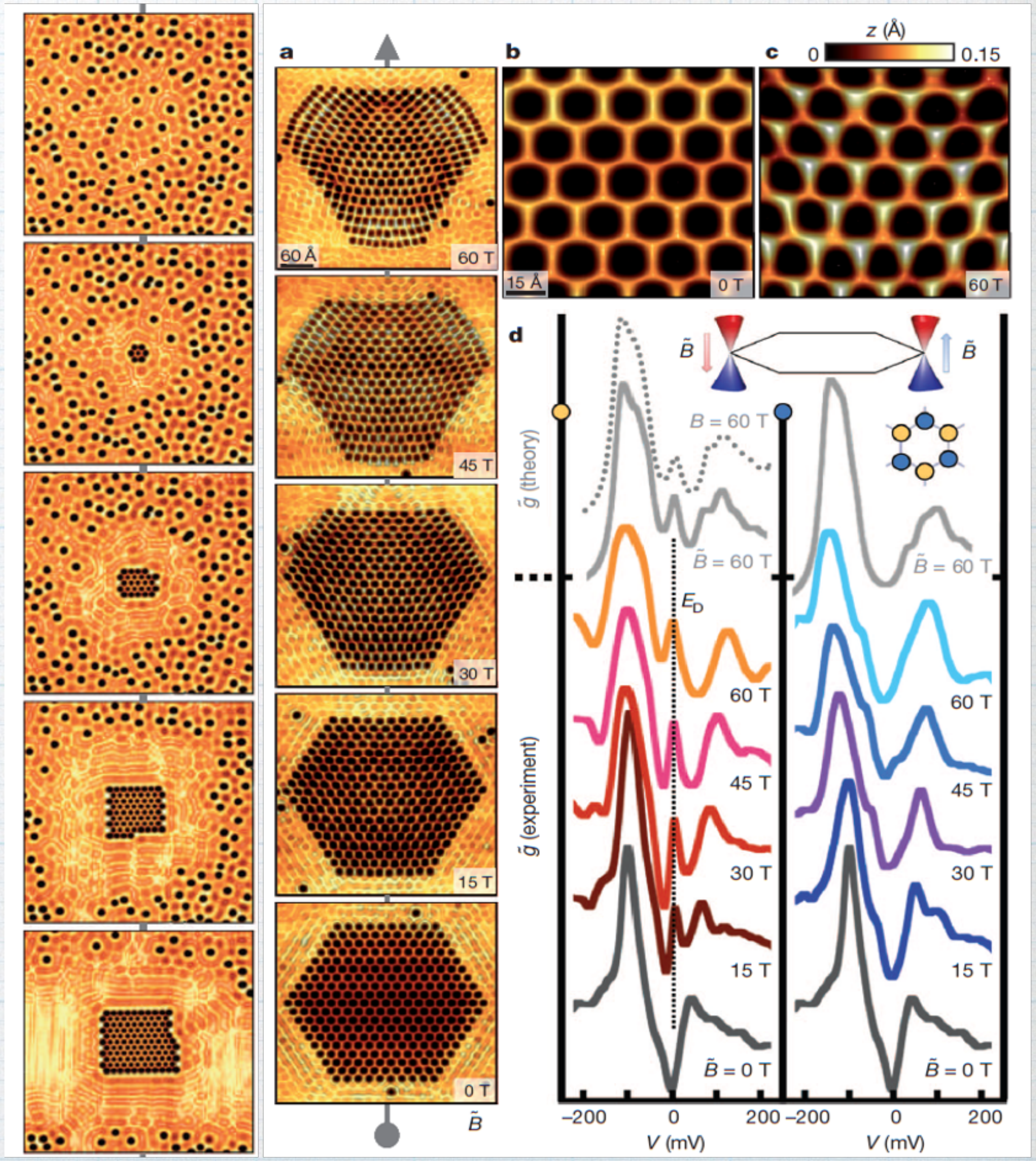
Pseudo Landau Levels



Nat Commun 3, 823 (2012)



Nano Lett. 2017, 17, 2240–2245



K. K. Gomes, et. al , Nature,483 306 (2012)

Starined BLG: Tight-binding Hamiltonian

$$H = \sum_{i,l}\{\epsilon_i{}^a a_i^{l\dagger} a_i^l + \epsilon_i{}^b b_i^{l\dagger} b_i^l\}$$

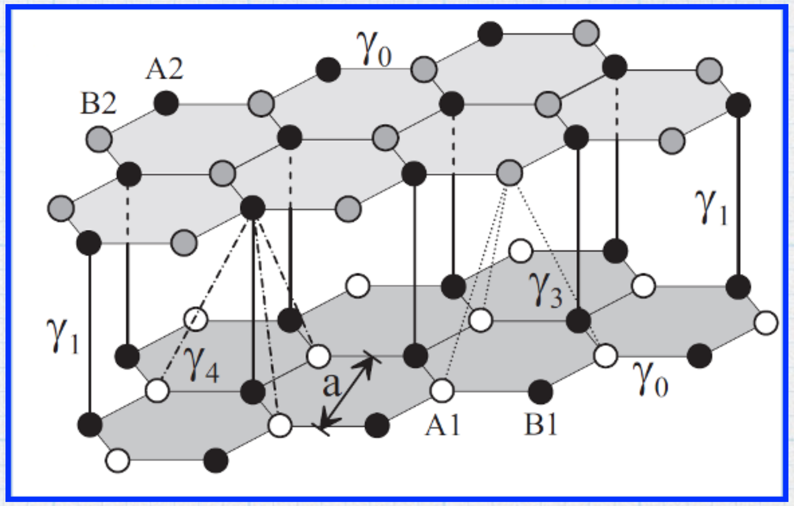
$$- \sum_{<ij>,l} \{\gamma_0^{ij} e^{\phi_{ij}} a_i^{l\dagger} b_j^l + H.c.\}$$

$$- \sum_{i}\{\gamma_1^{ij} a_i^{2\dagger} b_i^1 + H.c.\}$$

$$- \sum_{<ij>} \{\gamma_3^{ij} e^{\phi_{ij}} a_i^{1\dagger} b_j^2 + H.c.\}$$

$$\phi_{ij} = \frac{e}{\hbar}\int_i^j \vec{A}.\vec{dr}$$

$$\epsilon_i = (-1)^l \frac{u}{2}$$

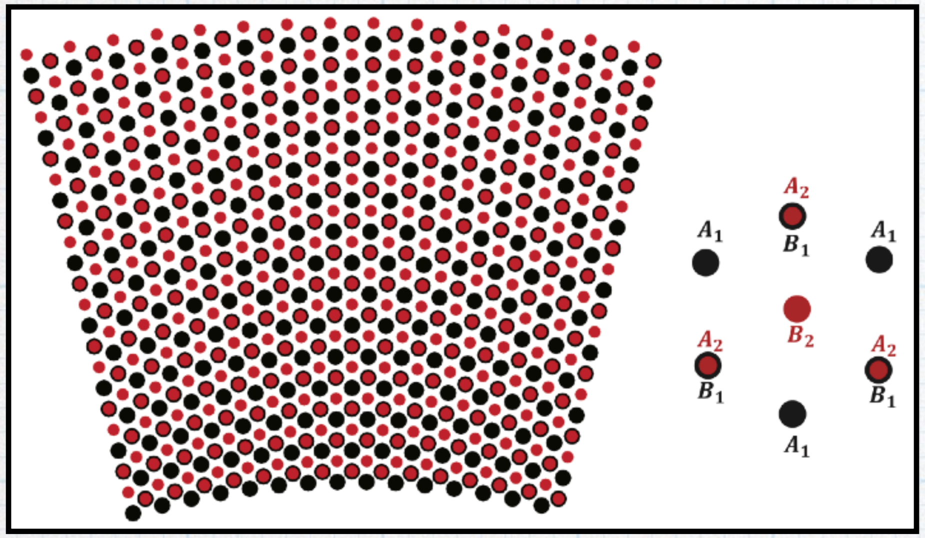


$$\gamma_0^{ij} = \gamma_0 e^{-\beta_0(\frac{d}{a_0}-1)} \quad , \quad \gamma_1^{ij} = \gamma_1 e^{-\beta_1(\frac{d}{c_0}-1)}$$

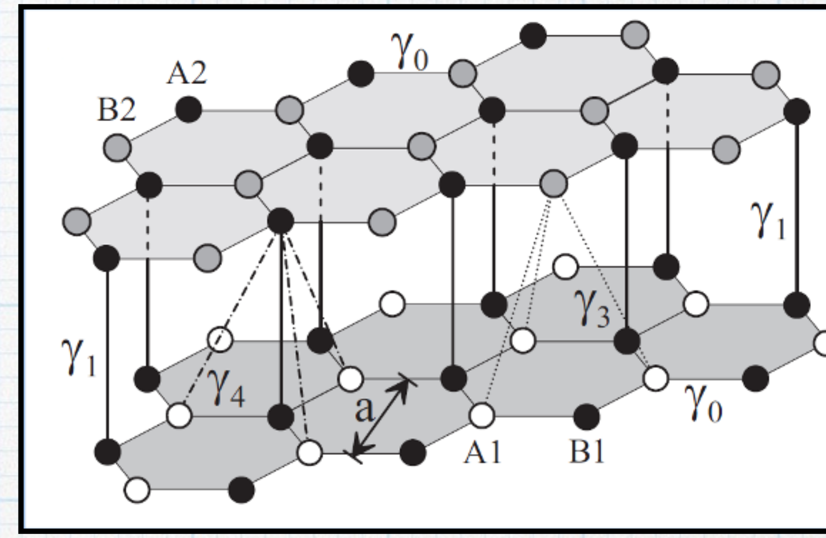
$$\gamma_3^{ij} = X\left[\gamma_0(\frac{d_\parallel}{d})^2 e^{-\beta_0(\frac{d}{\tilde{c}_0}-1)} + \gamma_1(\frac{d_\perp}{d})^2 e^{-\beta_1(\frac{d}{\tilde{c}_0}-1)}\right]$$

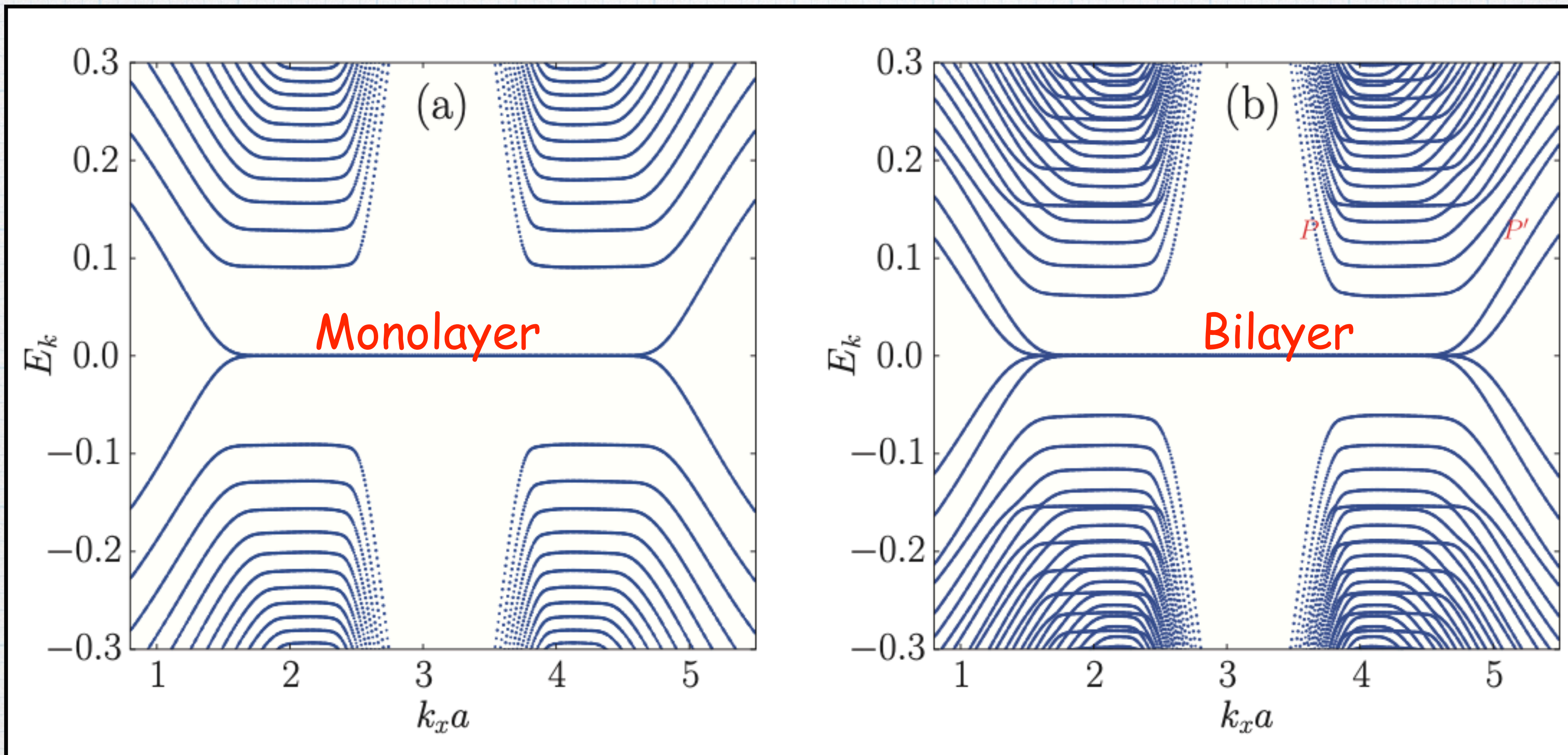
HR and Reza Asgari, Phys. Rev. B 88, 035404 (2013)

PLL in arc-shaped Bilayer Graphene



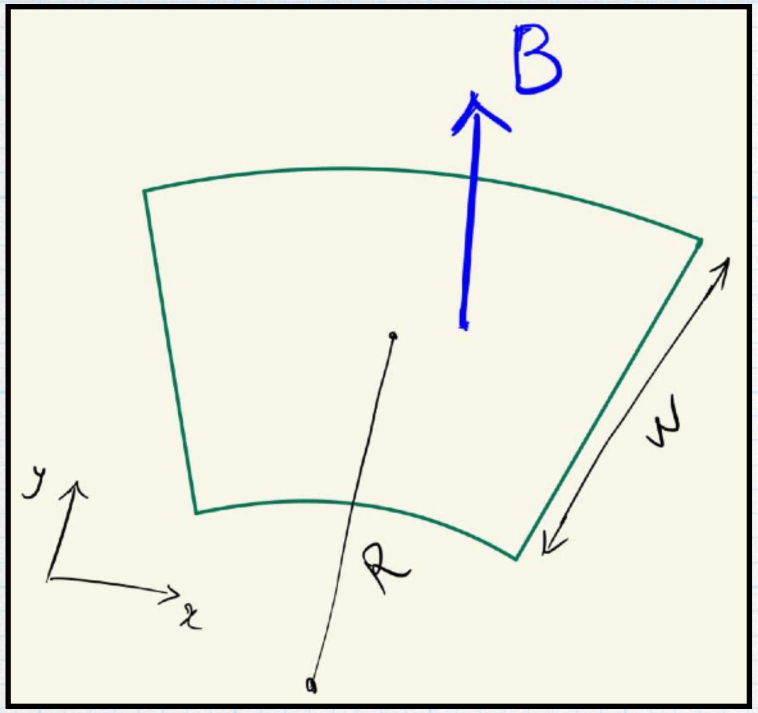
$$(u_x, u_y) = \left(\frac{xy}{R}, -\frac{x^2}{2R}\right)$$

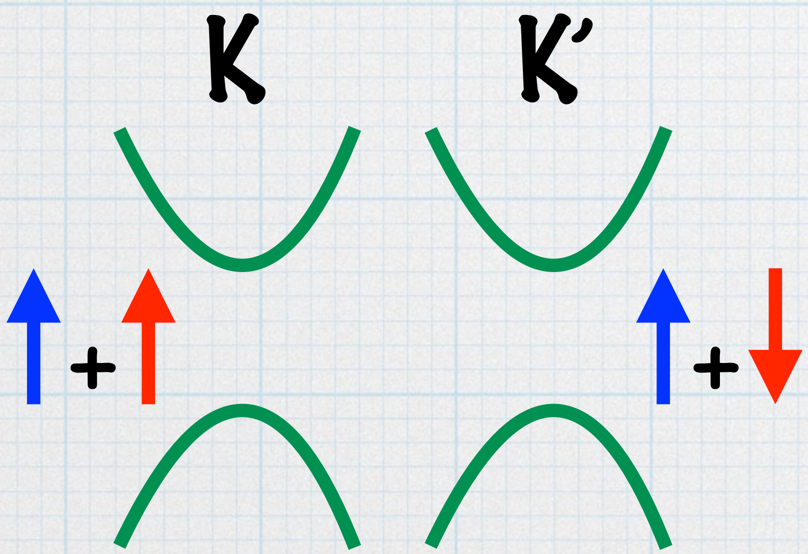


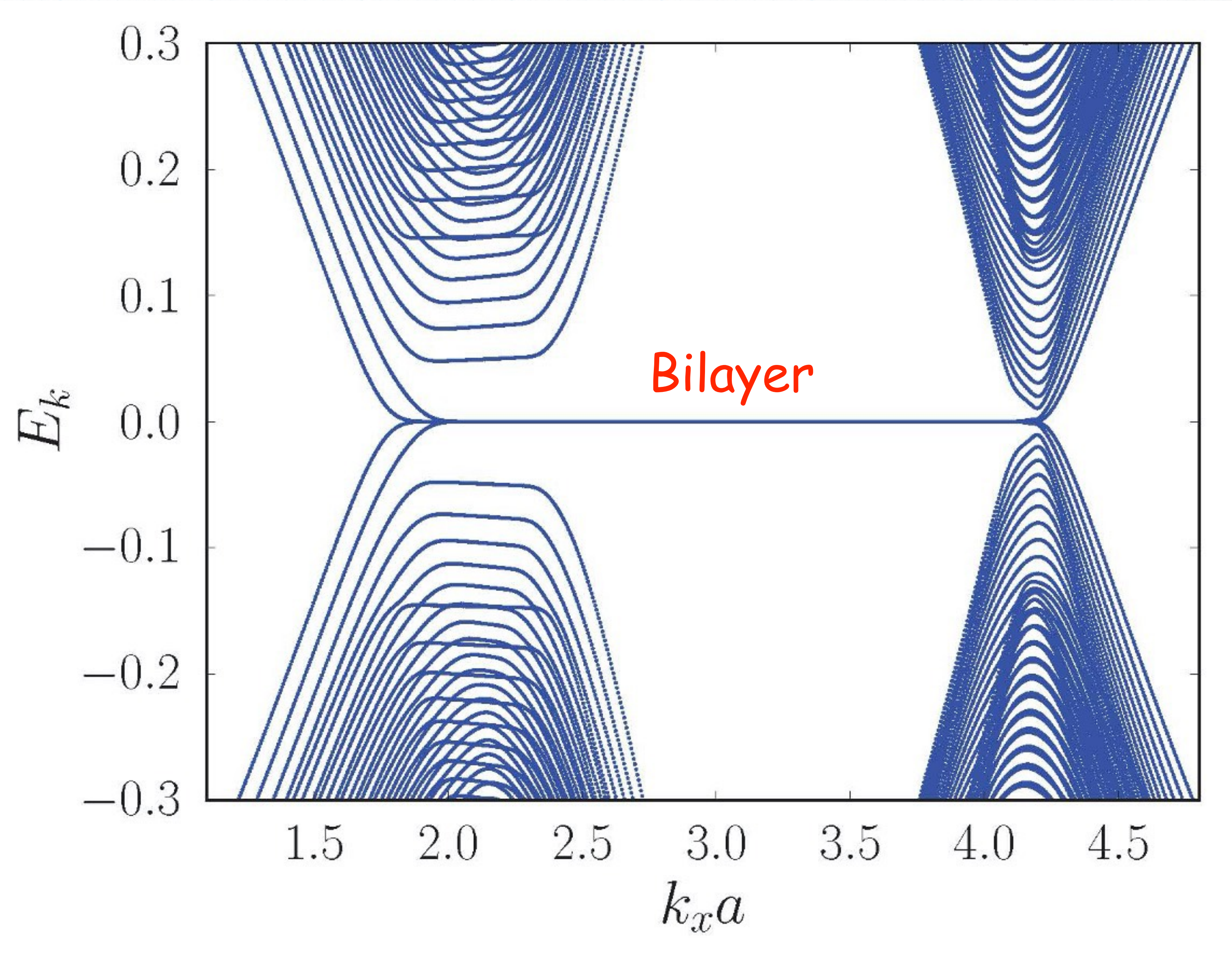


HR and Reza Asgari, Phys. Rev. B 88, 035404 (2013)

Real B + Pseudo B

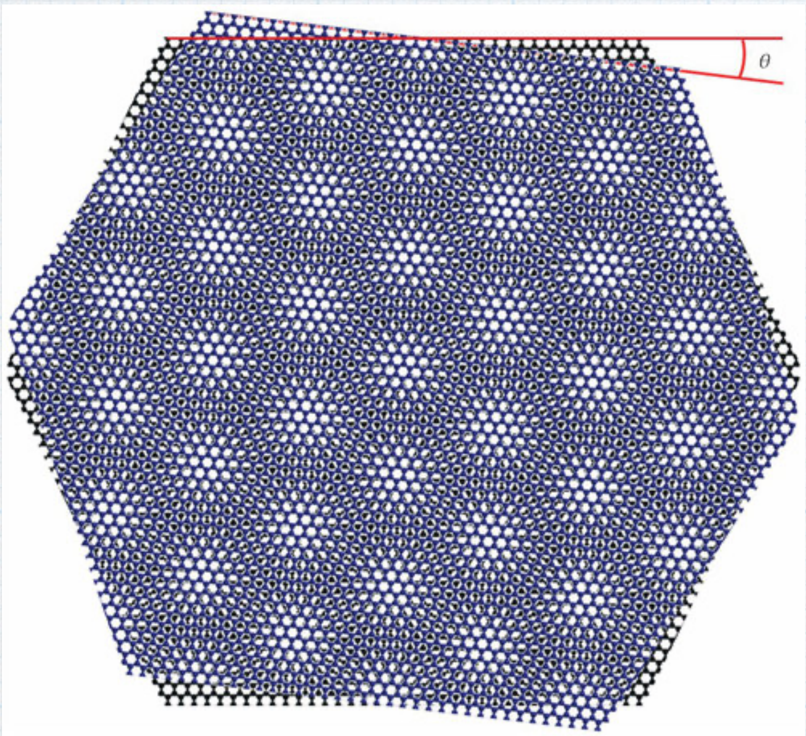






HR and Reza Asgari, Phys. Rev. B 88, 035404 (2013)

Relative twist of layers



PNAS July 26, 2011 108 (30) 12233-12237

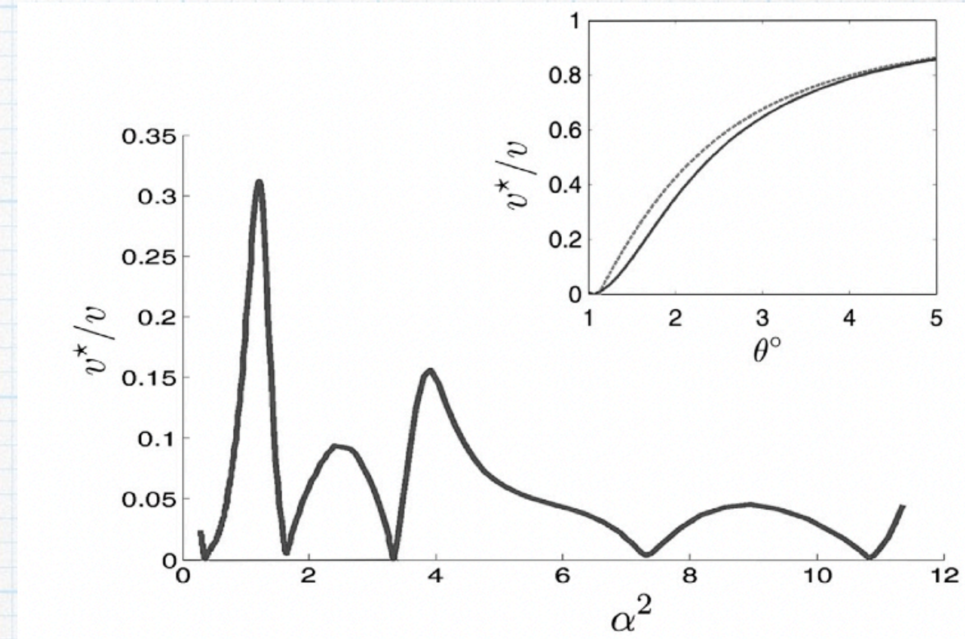
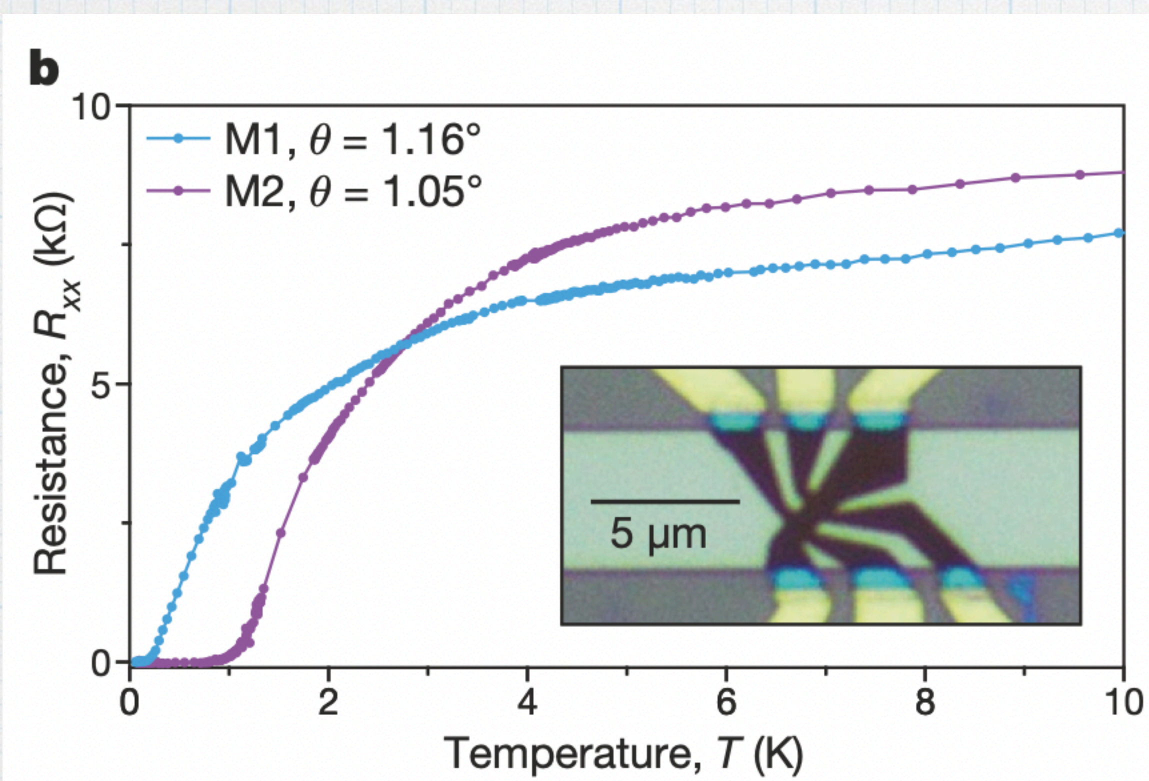
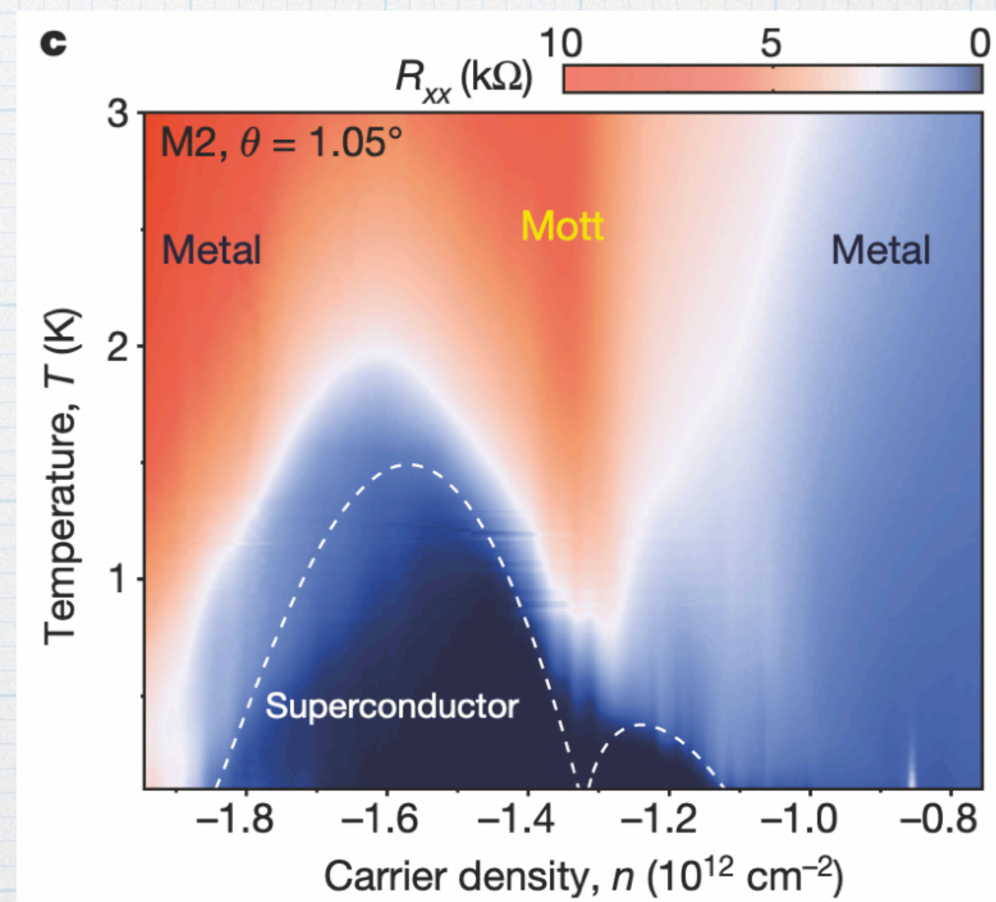


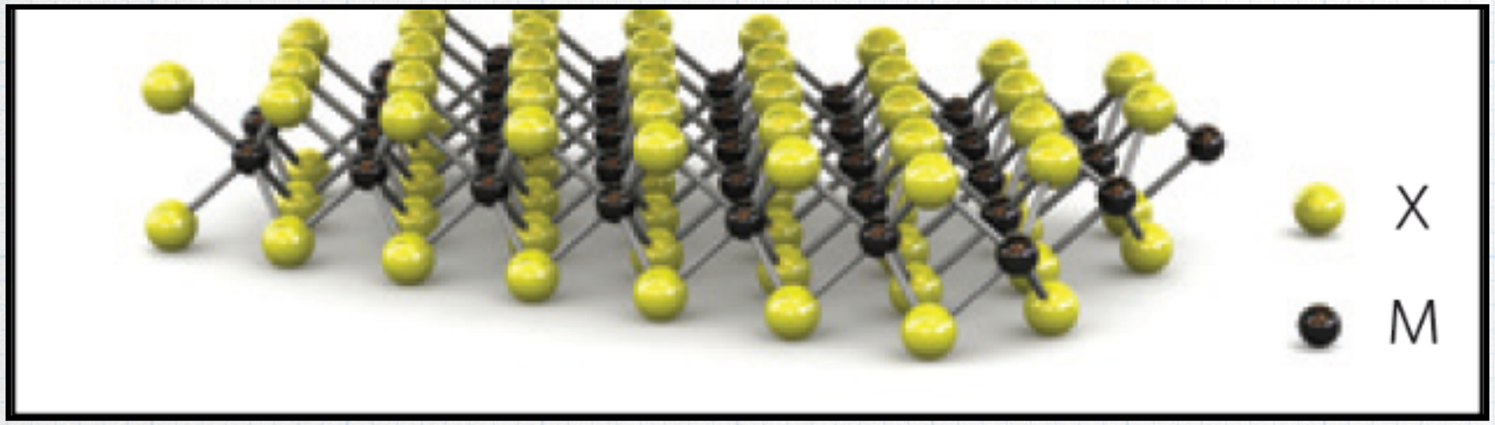
Fig. 4. Renormalized Dirac-point band velocity. The band velocity of the twisted bilayer at the Dirac point $v^{\star}$ is plotted vs. α^2, where $\alpha = w/vk_\theta$ for $0.18° < \theta < 1.2°$. The velocity vanishes for $\theta \approx 1.05°$, 0.5°, 0.35°, 0.24°, and 0.2°. (*Inset*) The renormalized velocity at larger twist angles. The solid line corresponds to numerical results and dashed line corresponds to analytic results based on the eight-band model.

Y. Cao et al. Nature 556,80 (2018), Nature 556,43 (2018)

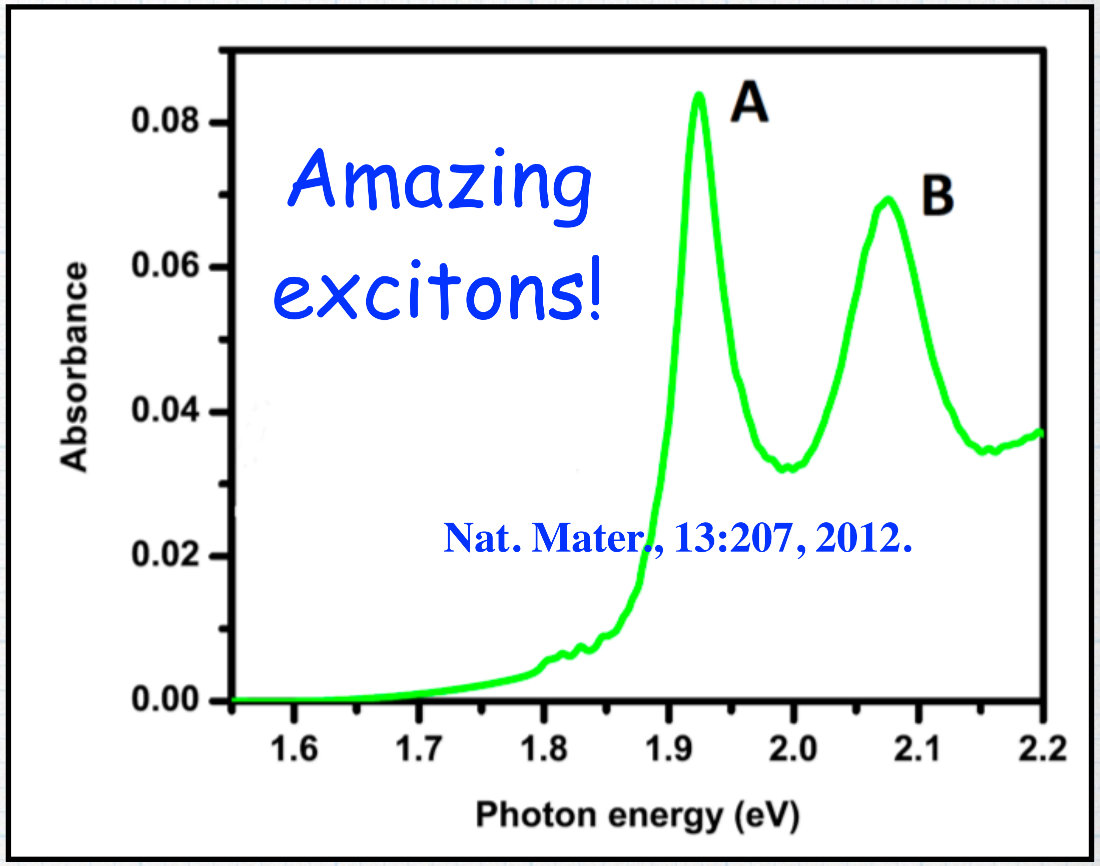


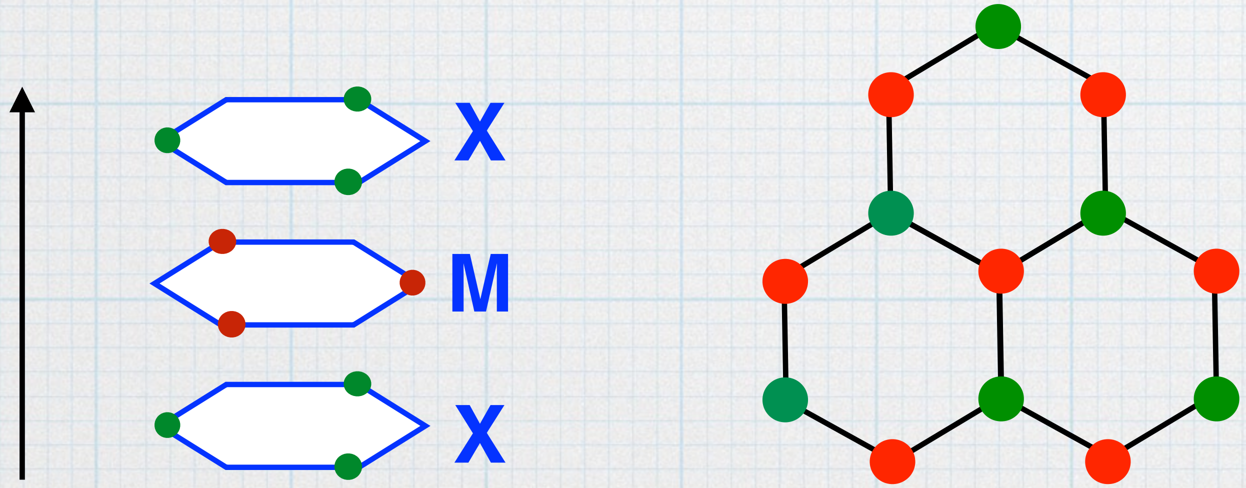


TMD: MoS2, WS2, …

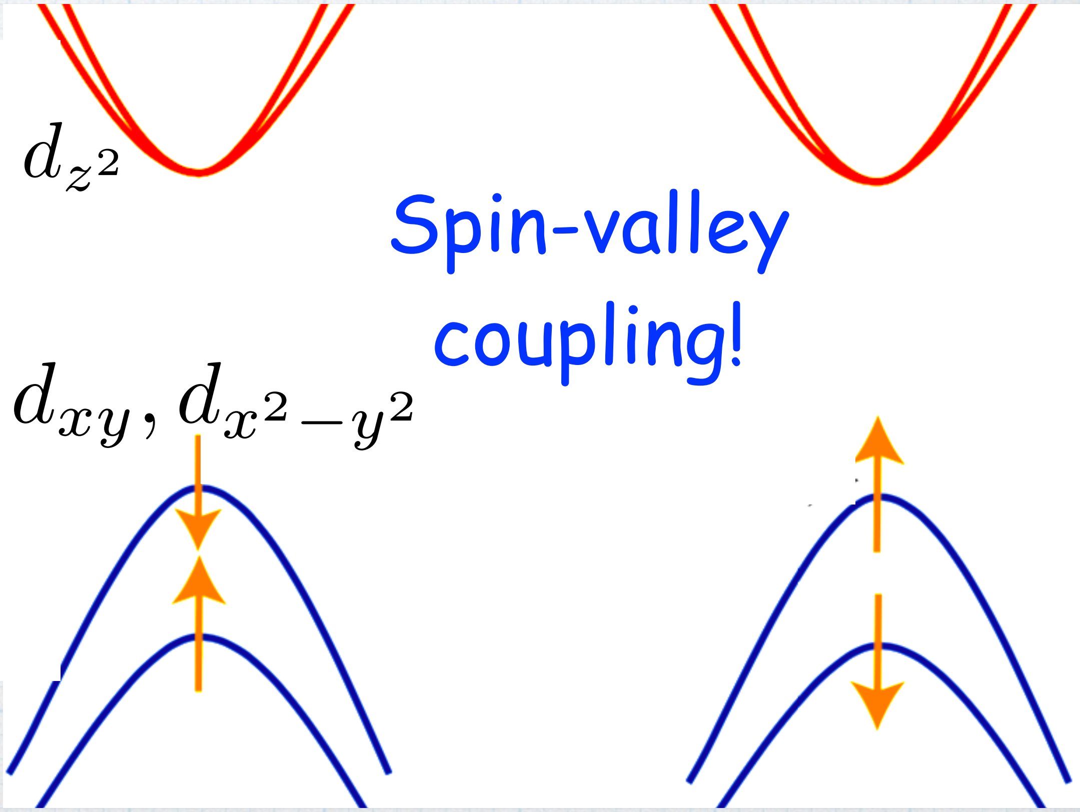


Nature Nanotech., 7:699, 2012.

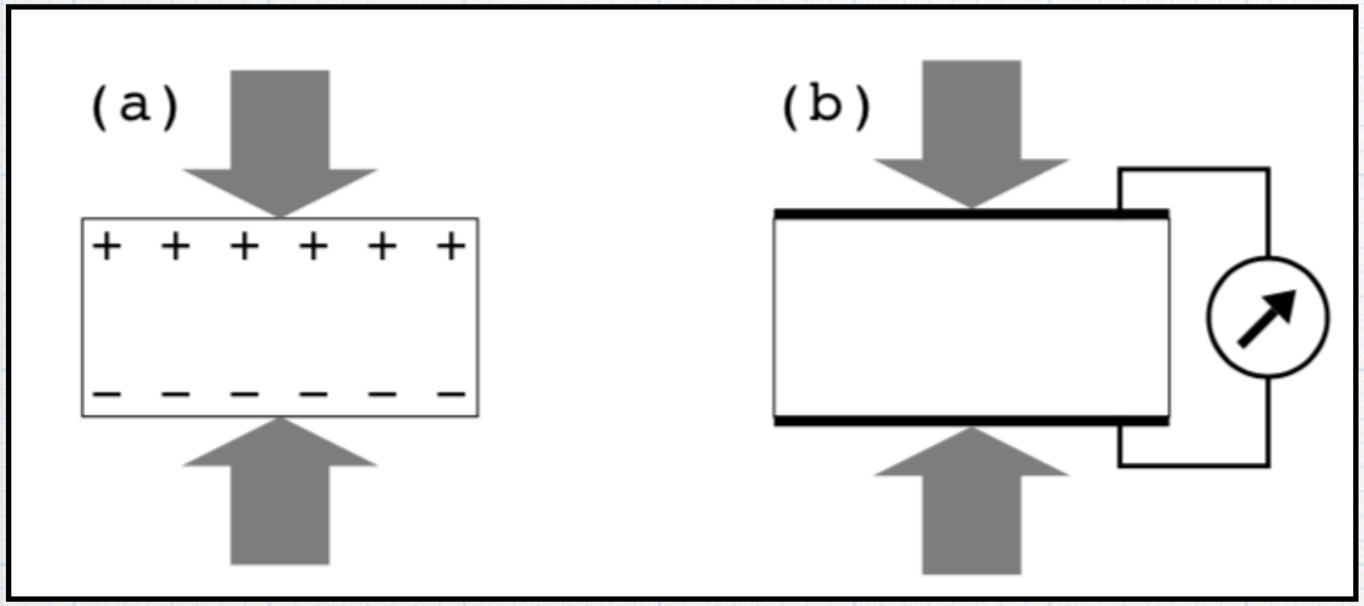


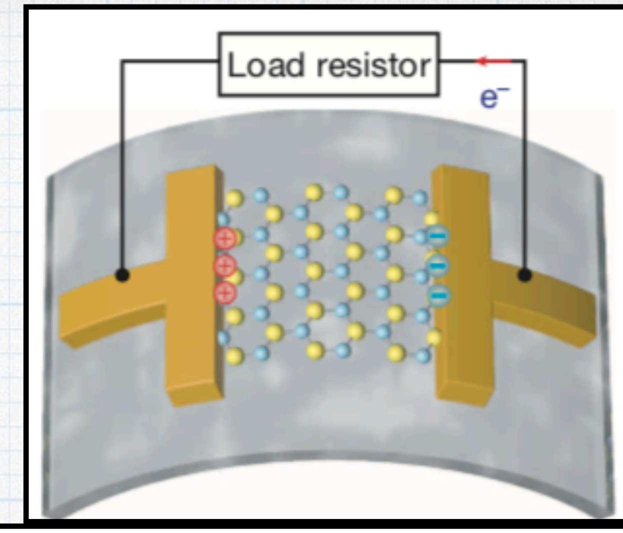


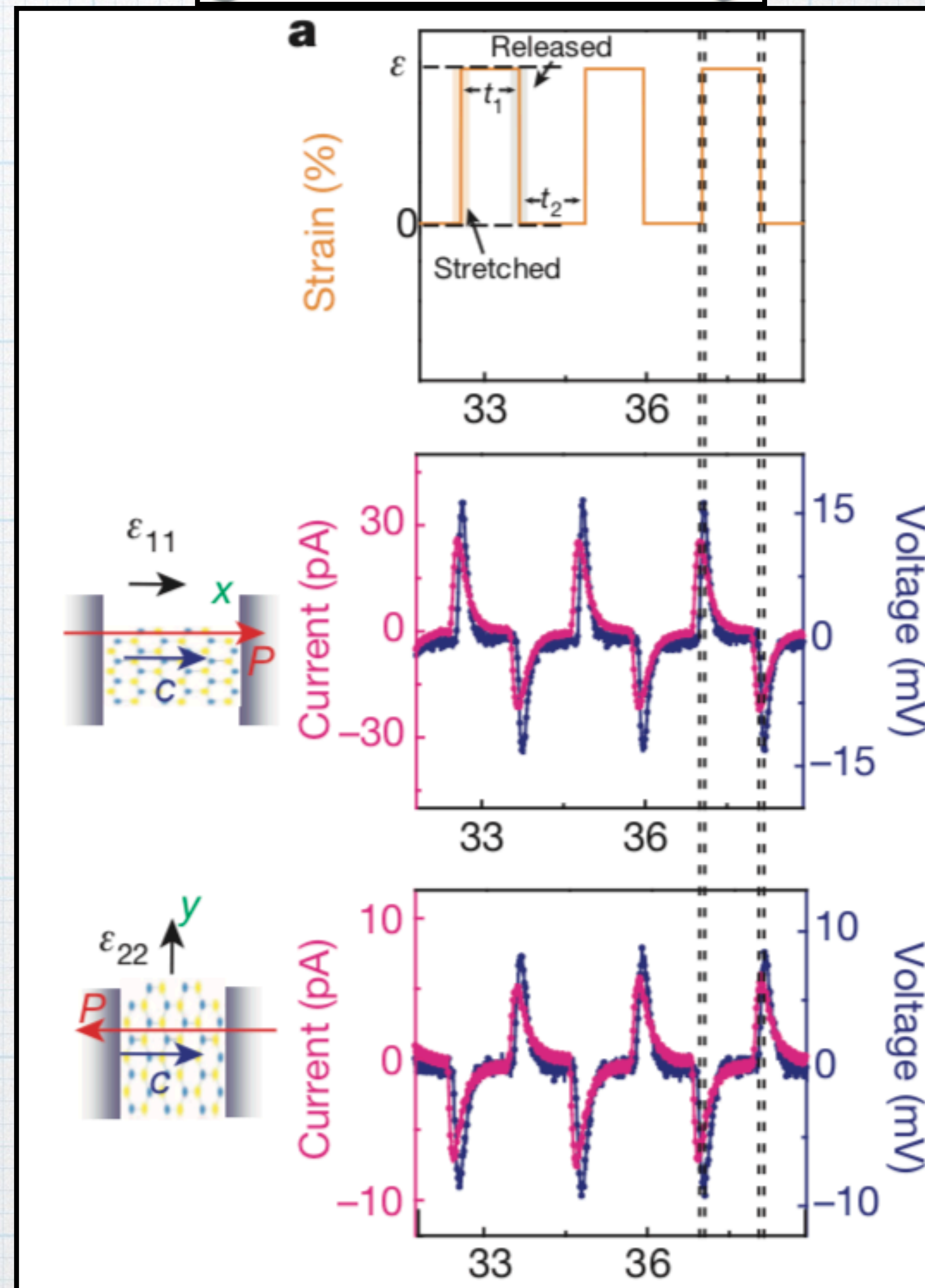
M: Mo, W   X: S, Se



Piezoelectricity







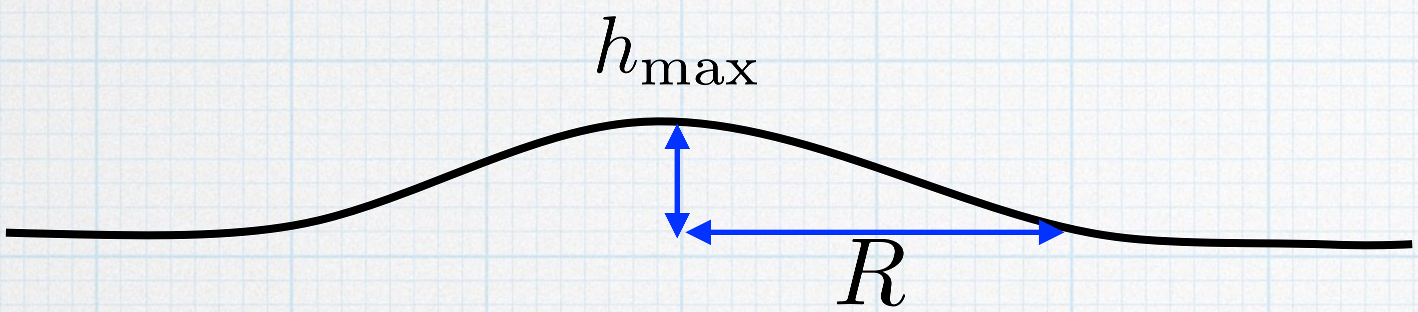
$$P = \gamma : \epsilon$$

Piezo (pressure) → Electricity

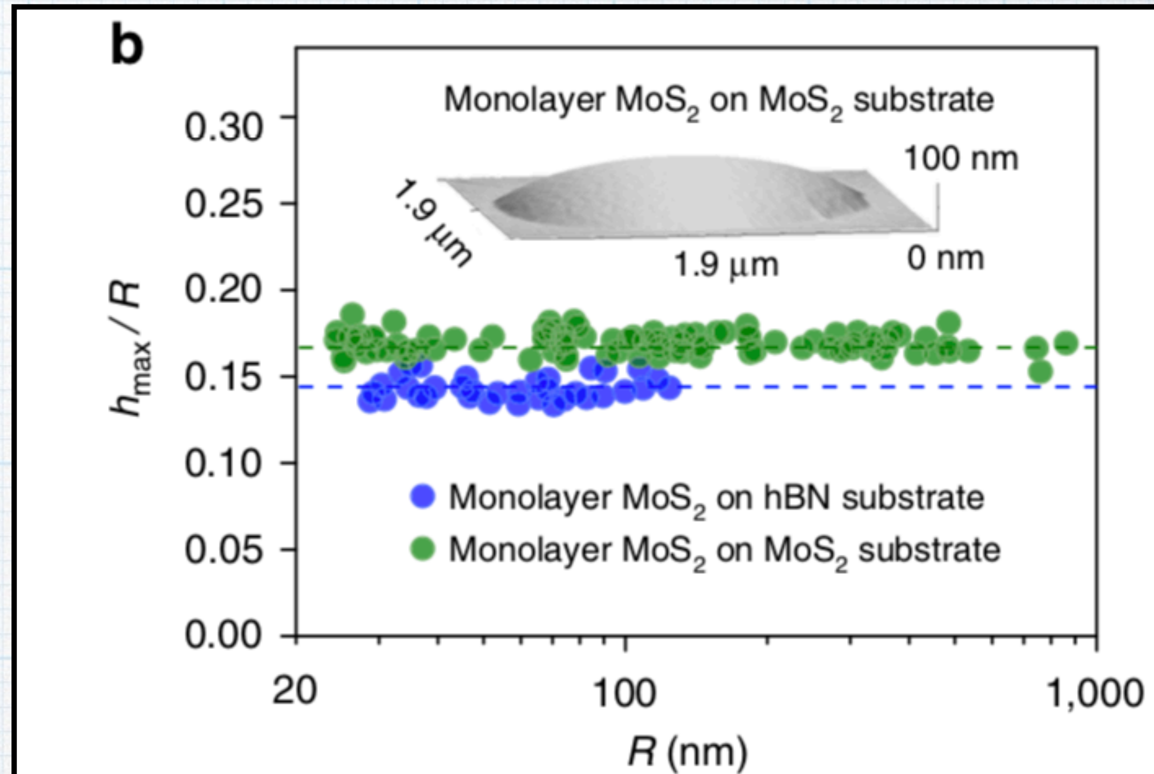
$$j(t) = \partial_t P(t)$$

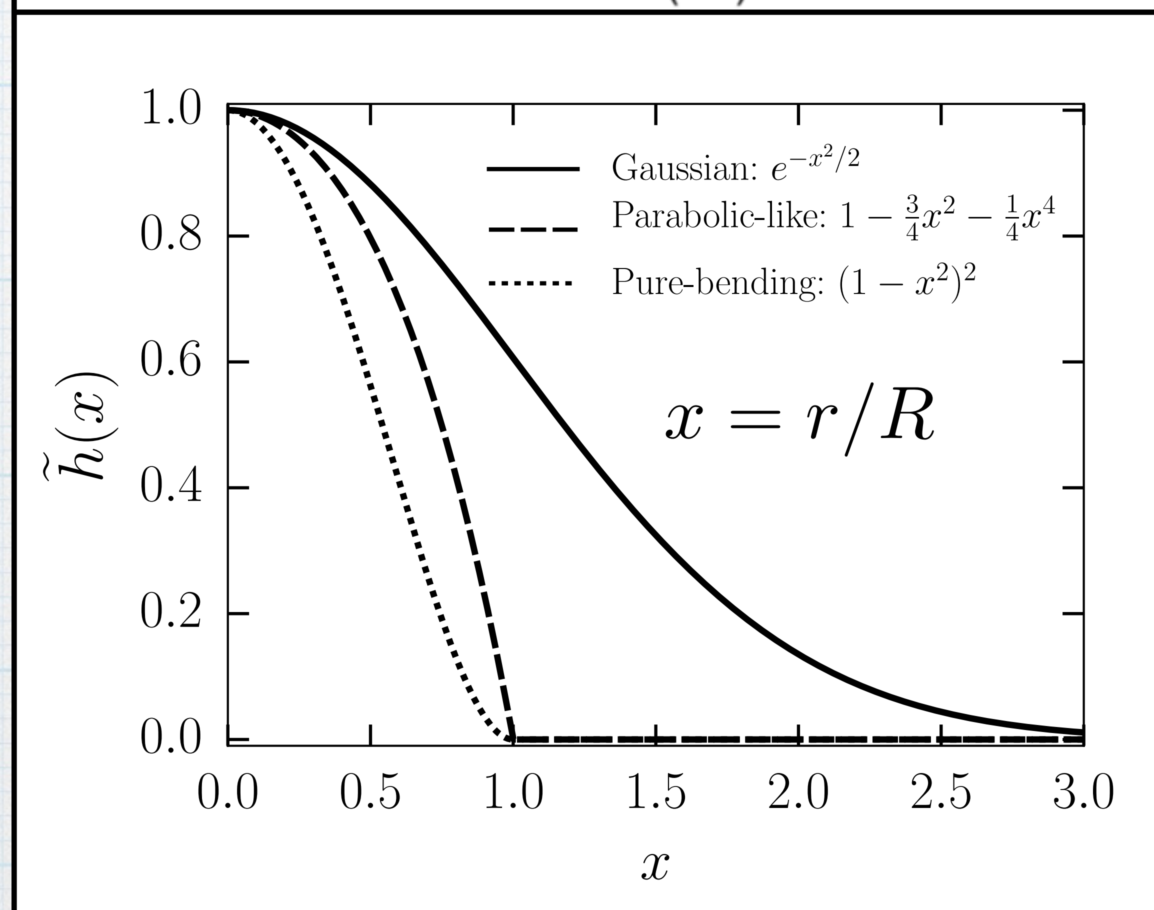
Nature 514, 470(2014).

Induced density in circular bubbles



Nat . Comm 7, 12587 (2016).





$$\boldsymbol{P} = \gamma_{yyy} \boldsymbol{\mathcal{A}} \times \hat{\boldsymbol{z}}$$

$$\boxed{\boldsymbol{P}(\boldsymbol{r}) = p(r)[\hat{\boldsymbol{r}} \sin(3\theta) + \hat{\boldsymbol{\theta}} \cos(3\theta)]}$$

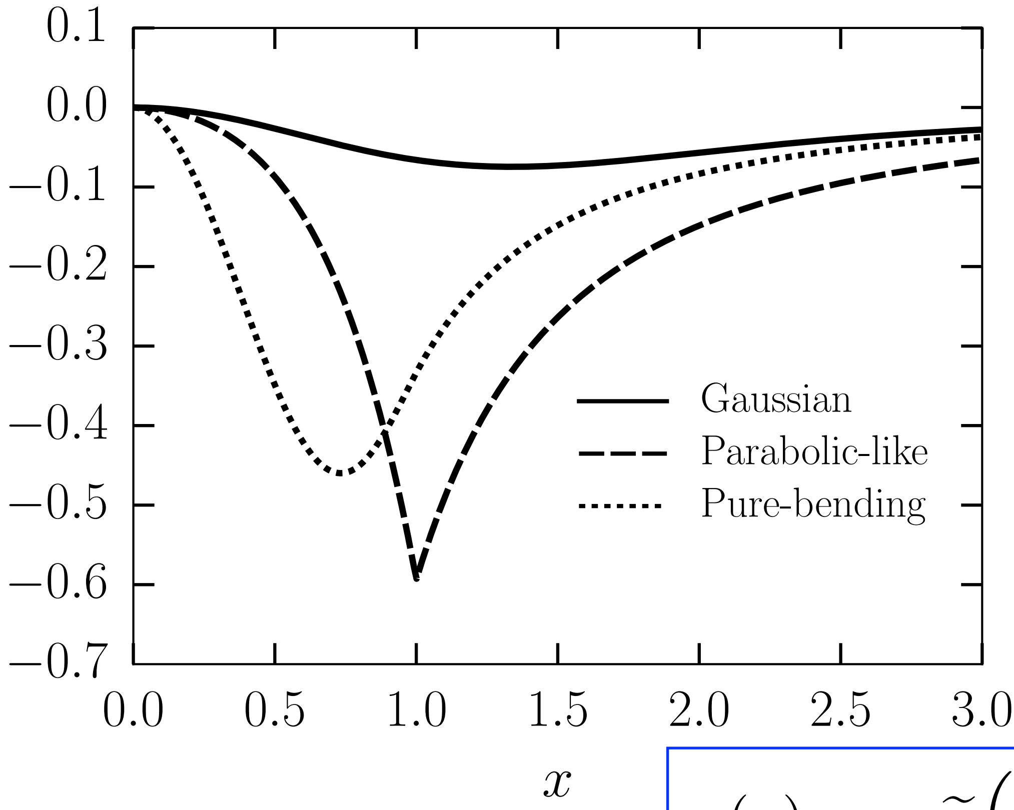
$$p(r) = \gamma \left\{ \frac{u(r)}{r} - \frac{\partial u(r)}{\partial r} - \frac{1}{2}\left(\frac{\partial h(r)}{\partial r}\right)^2 \right\}$$

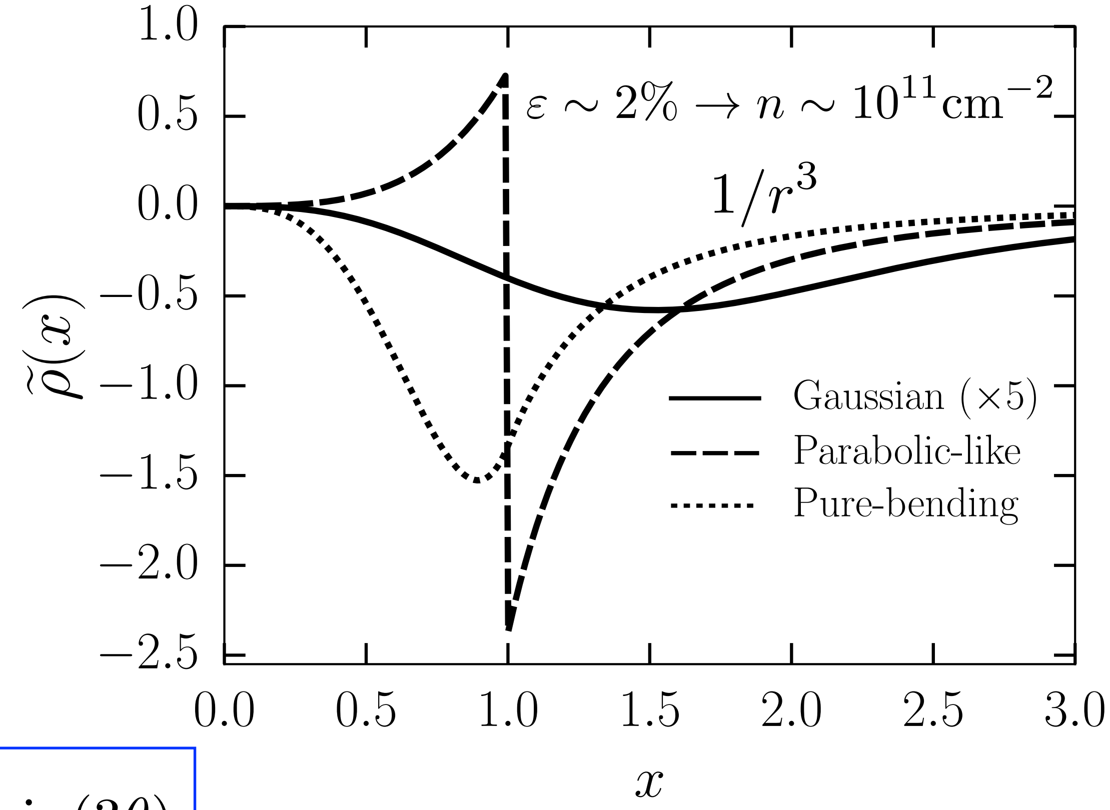
$$\rho(\boldsymbol{r}) = -\boldsymbol{\nabla} \cdot \boldsymbol{P}(\boldsymbol{r}) = -\gamma[\boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{r})]_z$$

$$\boxed{\rho(\boldsymbol{r}) = \left(\frac{p_0}{R}\right) \tilde{\rho}\left(\frac{r}{R}\right) \sin(3\theta)}$$

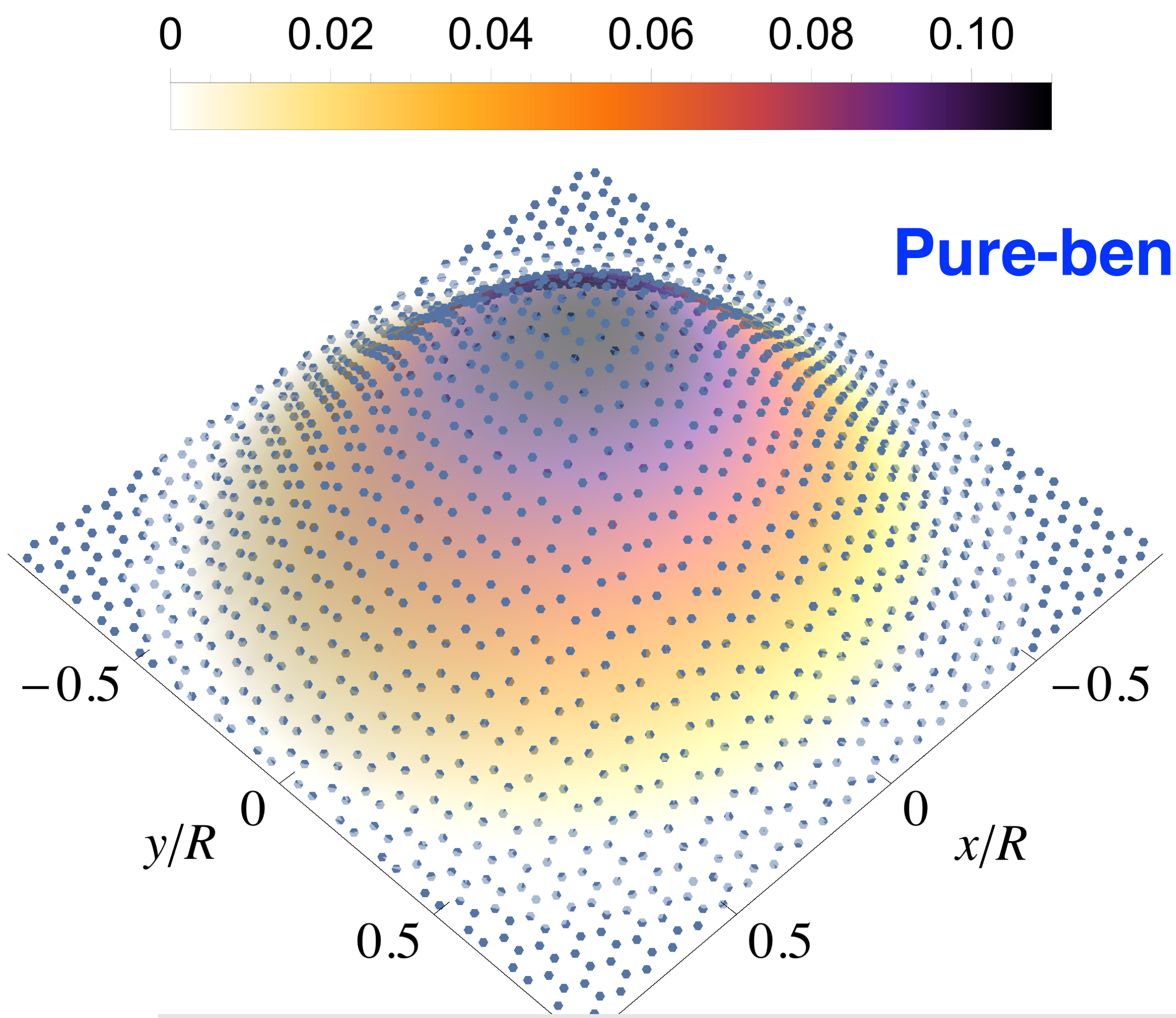
$$p_0 = \gamma(1+\nu) h_{\max}^2 / R^2$$

H.R., F. Guinea, M.Polini, R. Roldán, npj 2D Materials and Applications 2:15 (2018).

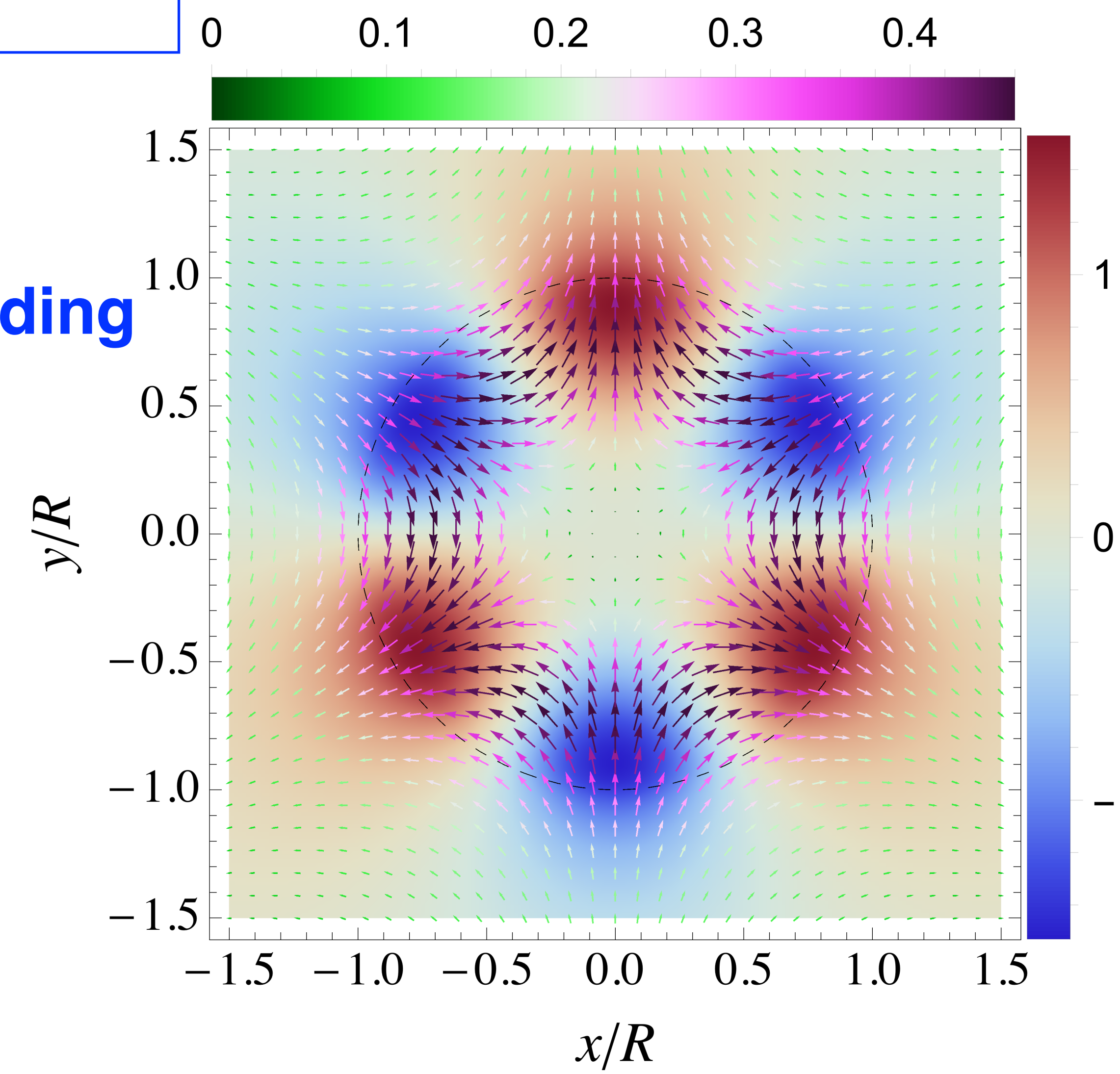




$$\boxed{\rho(\boldsymbol{r}) = \rho_0 \widetilde{\rho}\left(\frac{r}{R}\right)\sin(3\theta)}$$



Pure-bending



H.R., F. Guinea, M.Polini, R. Roldán, npj 2D Materials and Applications 2:15 (2018).

Summary

A. van der Waals layered materials provide a rich platform for nano-kirigami (origami) technology and flexible optoelectronic

B. 2D materials' electronic properties are highly sensitive to lattice deformation (strain): e.g. Pseudo Landau Levels

C. Relative rotation (twist) can lead us to exotic strongly correlated phases in 2D material's heterostructure

Thank you