Effective equations for Graphene

F. Biancalana

Heriot-Watt University, Edinburgh (UK)
&
Max Planck Institute for the Science of Light, Erlangen (DE)

SIF conference
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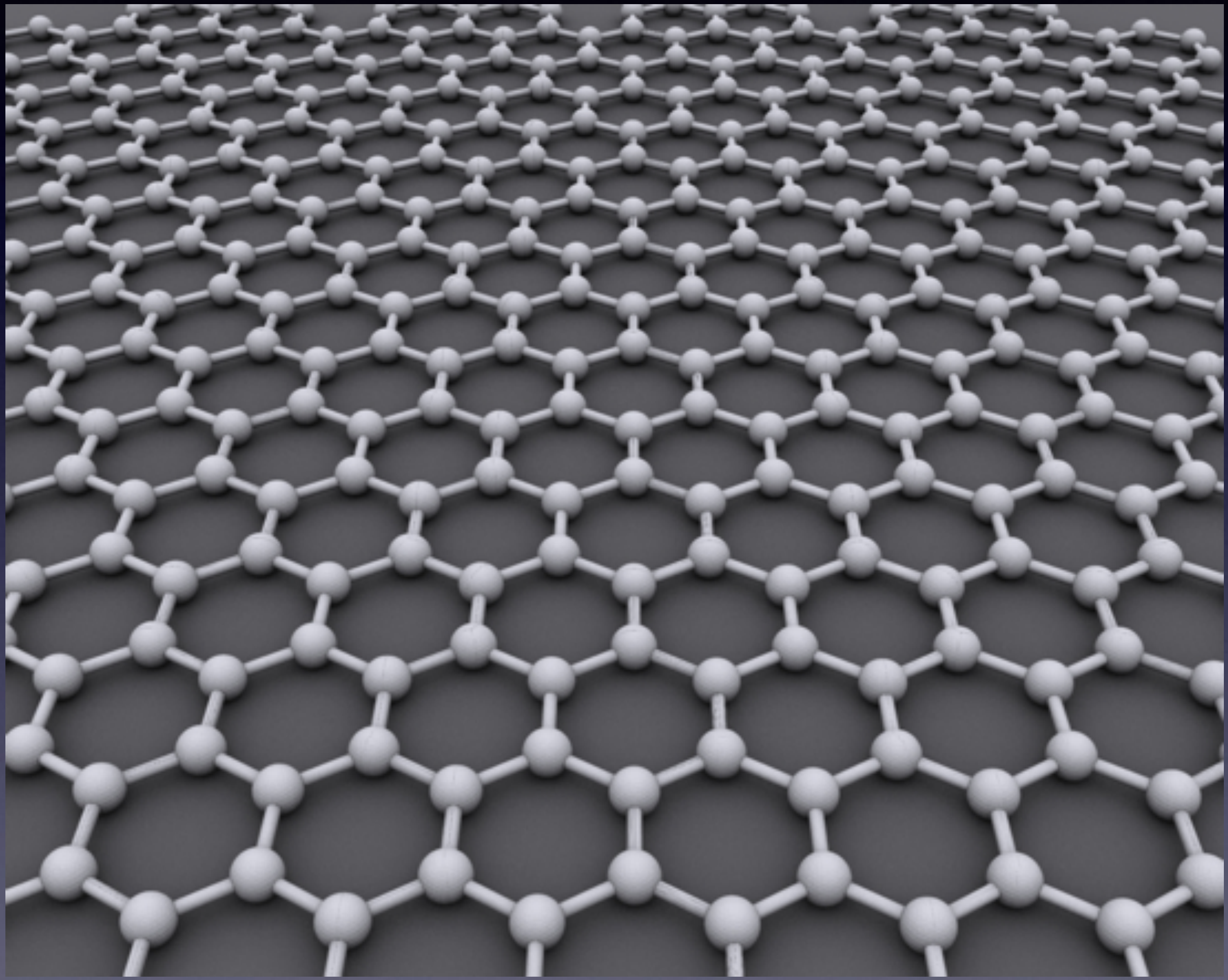
MAX-PLANCK-GESELLSCHAFT

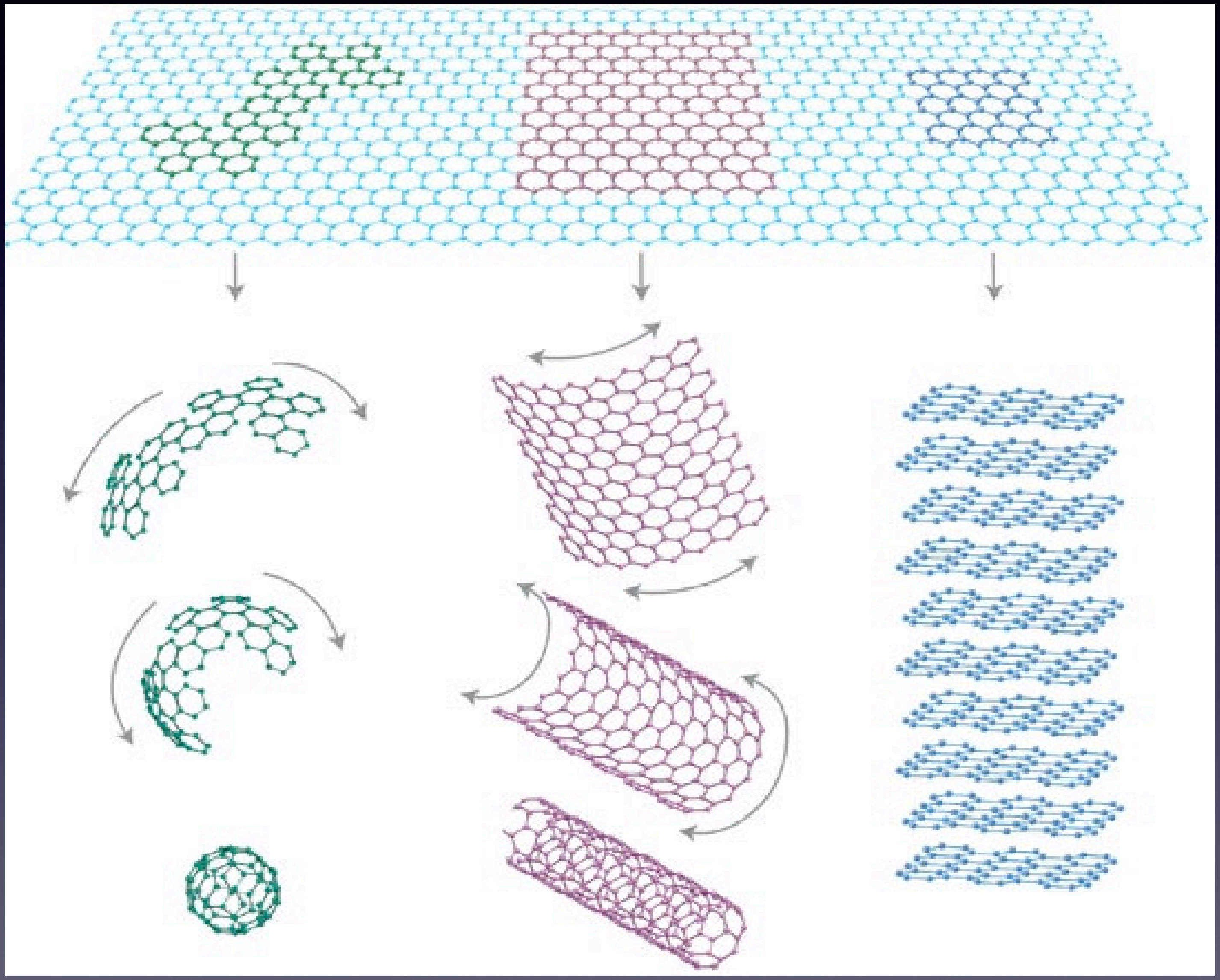
Graphene

- Single-layer 2D carbon-based material
- Honeycomb lattice
- Nobel 2010

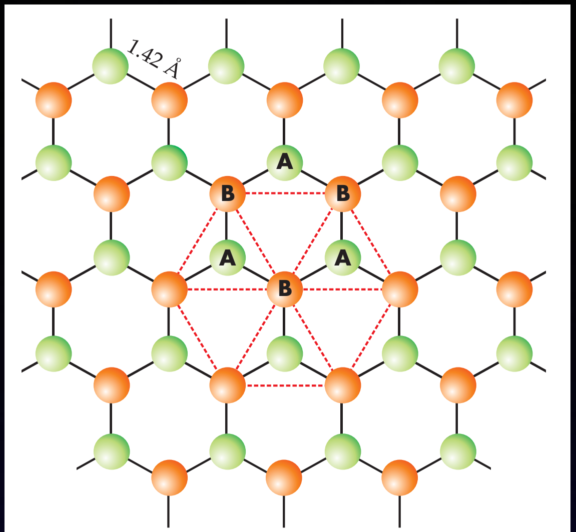


Carbon allotropes

- Carbon allows many different shapes to be engineered
- Bucky-balls, carbon tubes, stripes, etc…
- Very important for future electronic devices

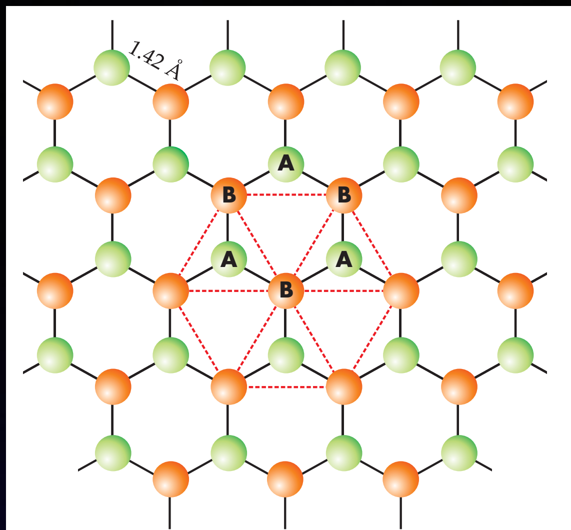


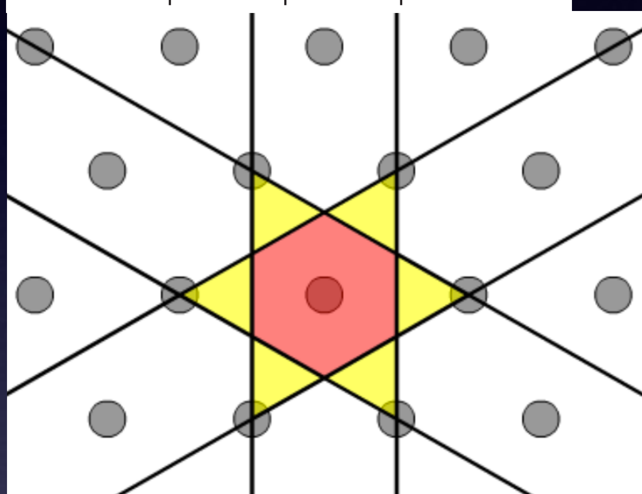
Graphene dispersion



$$H = -t \sum_{\langle i,j \rangle, \sigma=\uparrow,\downarrow} \left(a^{\dagger}_{\sigma,i} b_{\sigma,j} + h.c. \right) - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma=\uparrow,\downarrow} \left(a^{\dagger}_{\sigma,i} a_{\sigma,j} + b^{\dagger}_{\sigma,i} b_{\sigma,j} + h.c. \right)$$

Graphene dispersion





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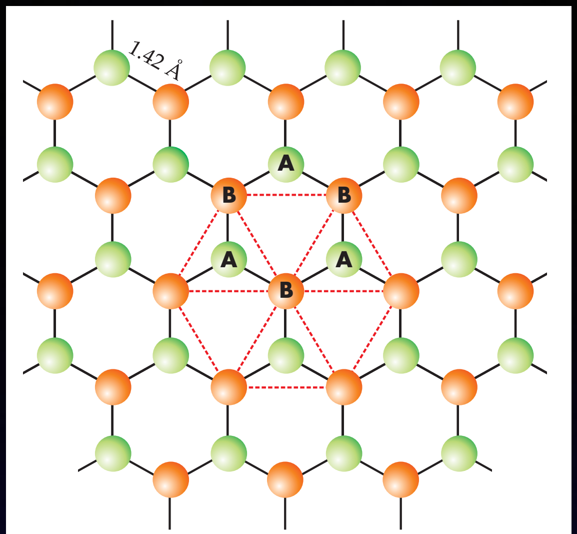
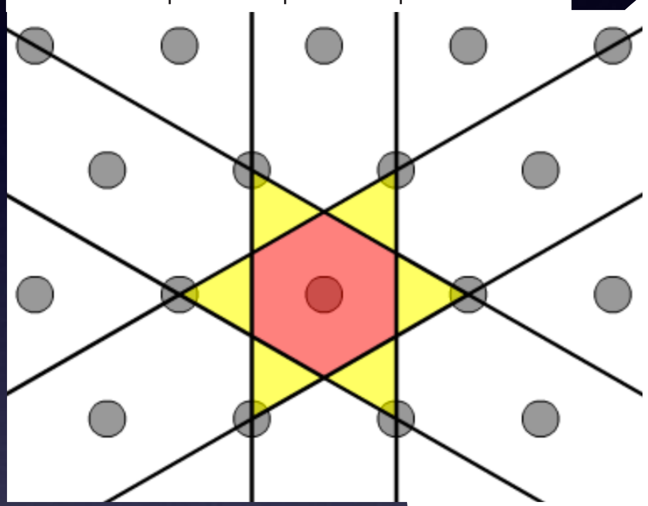
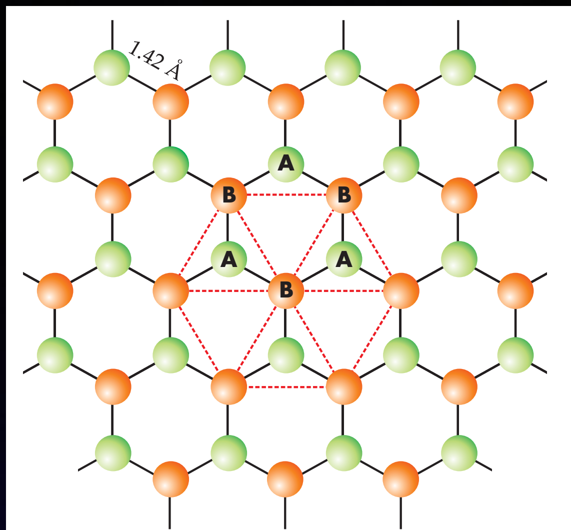
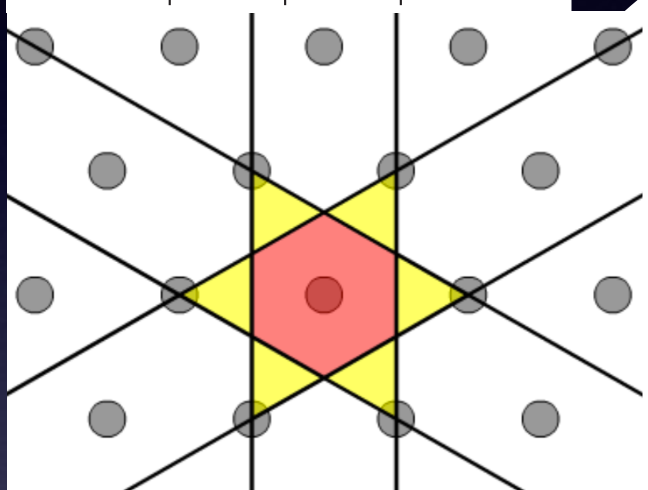




$$E = \pm\sqrt{\gamma_0^2\left(1 + 4\cos^2\frac{k_y a}{2} + 4\cos\frac{k_y a}{2}\cdot\cos\frac{k_x\sqrt{3}a}{2}\right)}$$

Graphene dispersion





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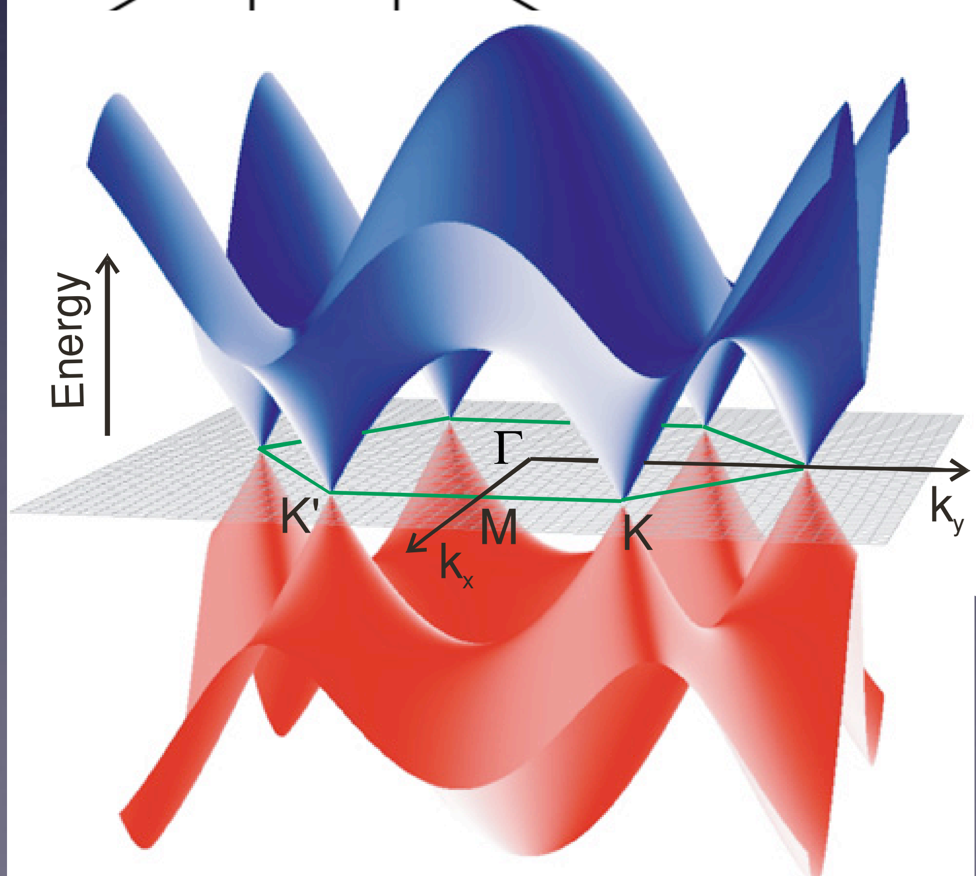

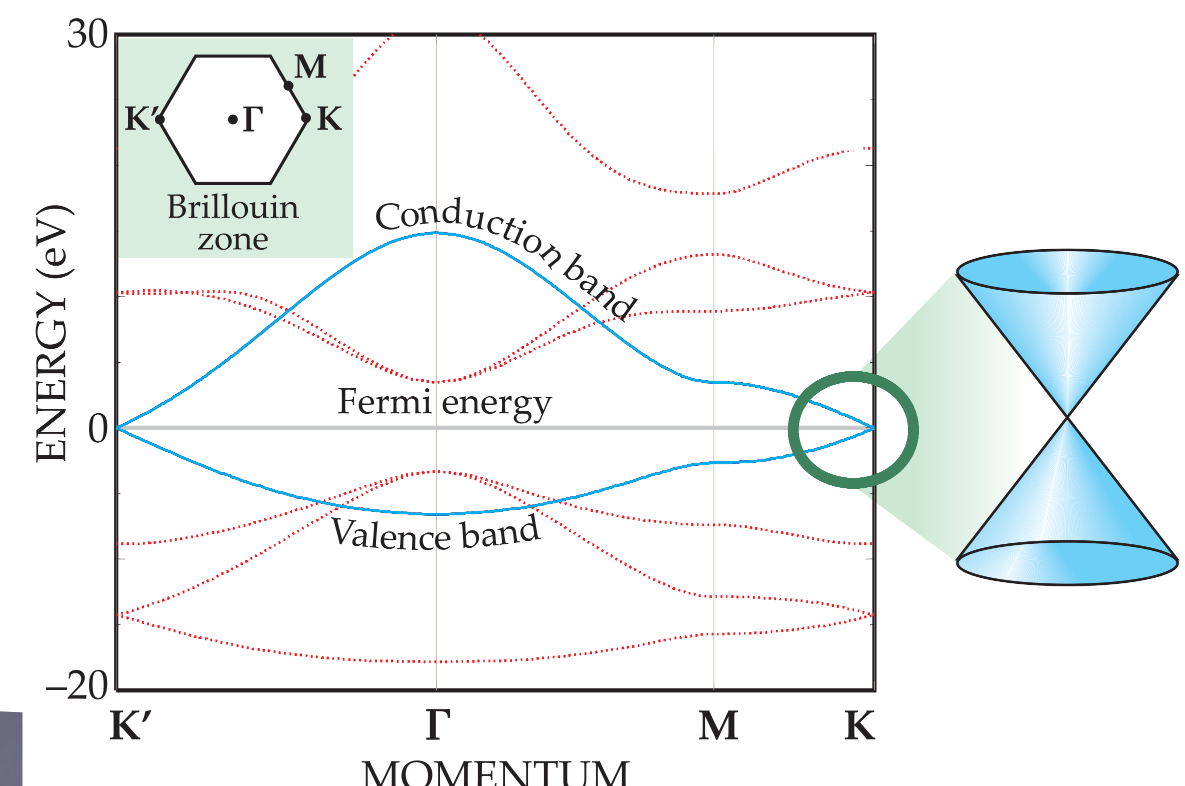

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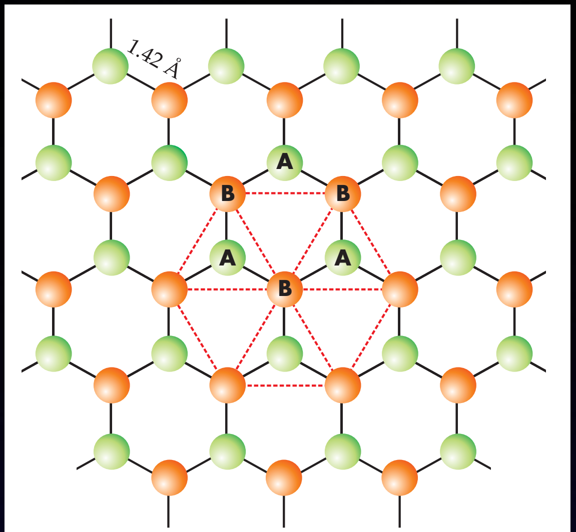

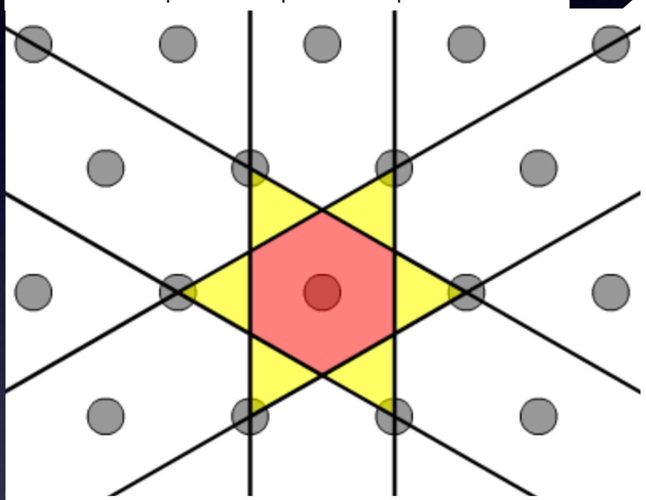

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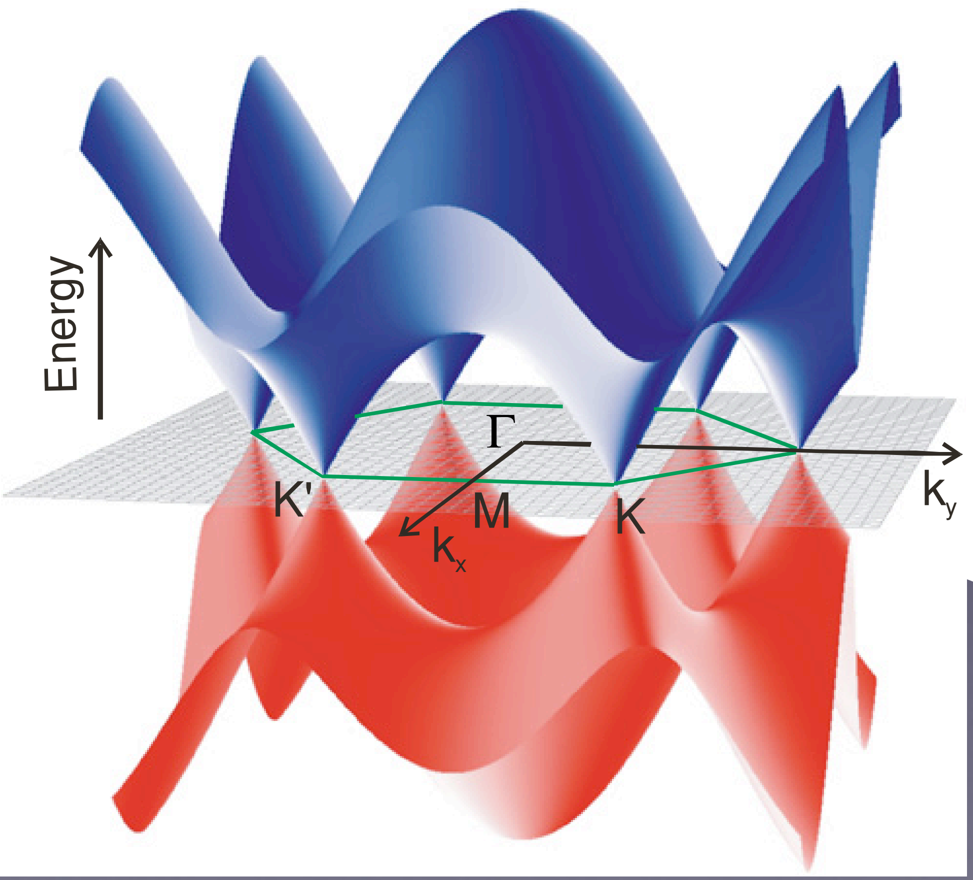
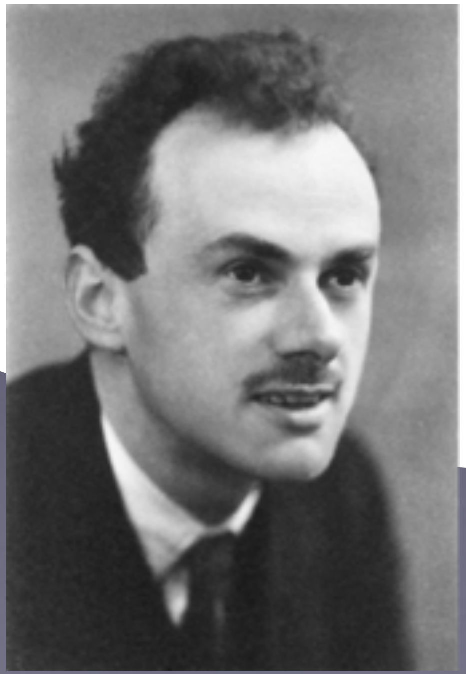
Dirac-Weyl equation
"charged neutrinos"

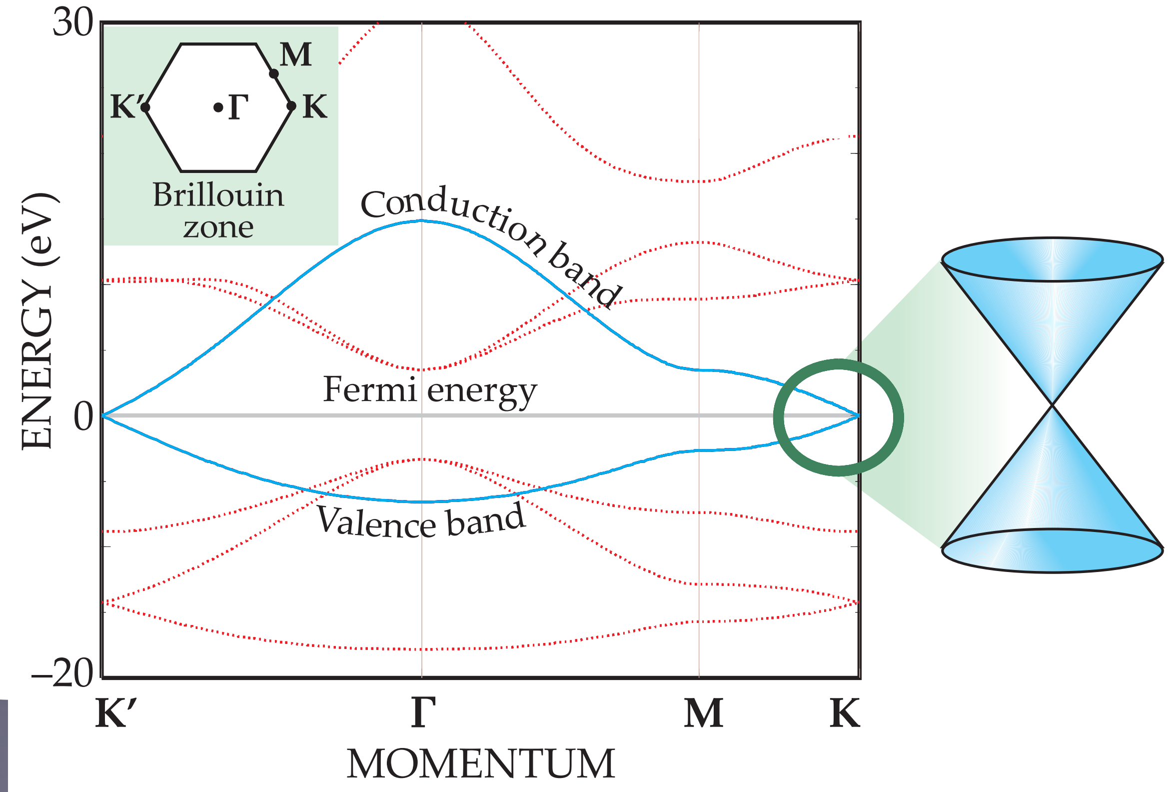
$$v_F\,\vec{\sigma}\cdot\nabla\psi(\mathbf{r}) \;=\; E\psi(\mathbf{r}).$$

$v_F \simeq 10^8\ cm/s$

$$E = \hbar v_F\sqrt{k_x^2 + k_y^2}$$







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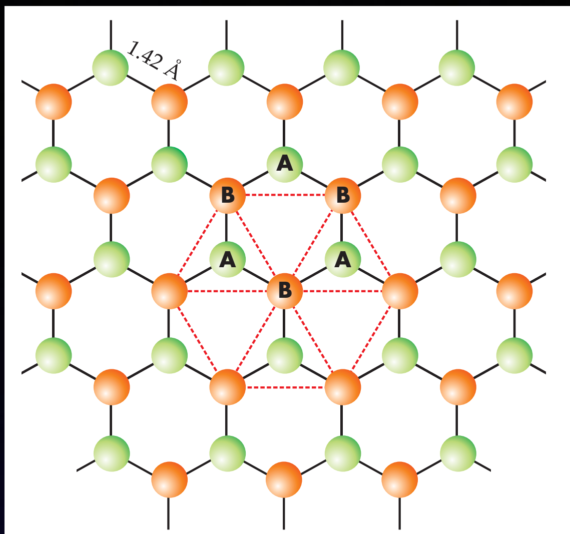

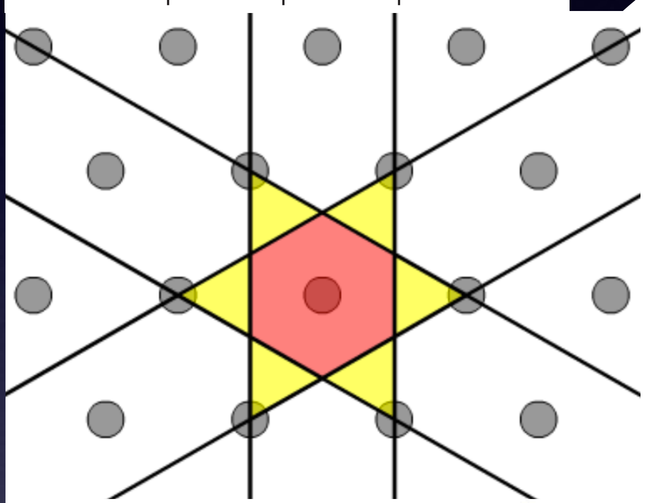

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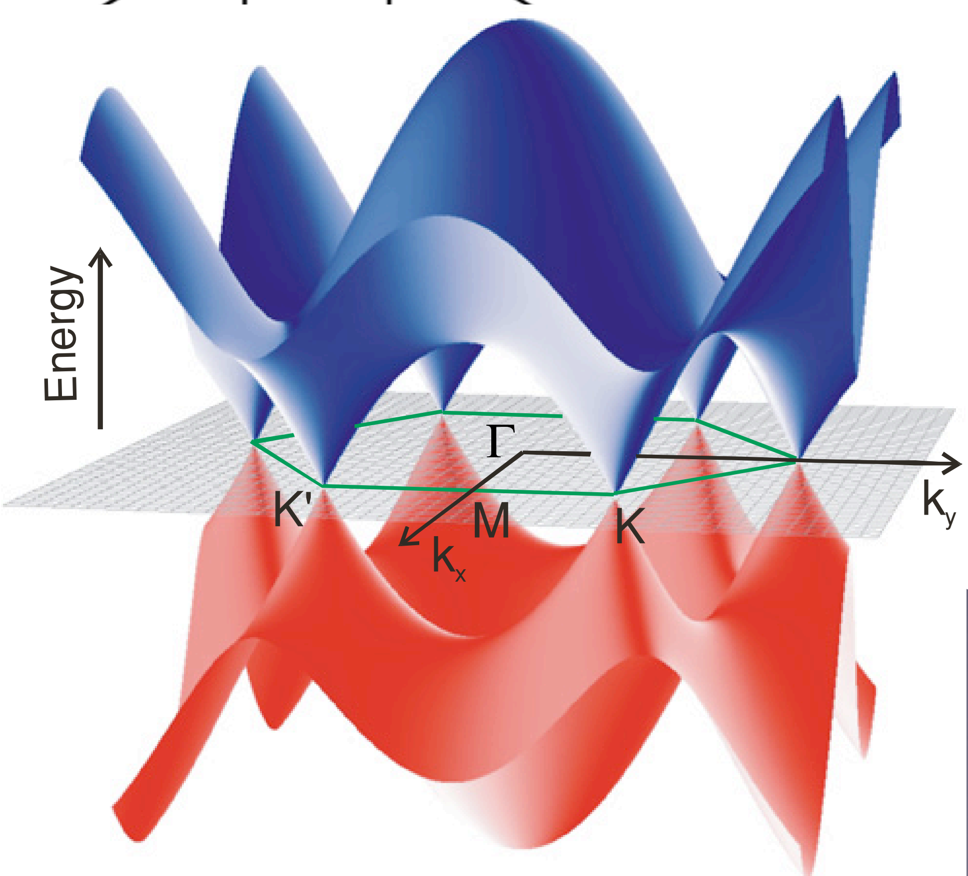
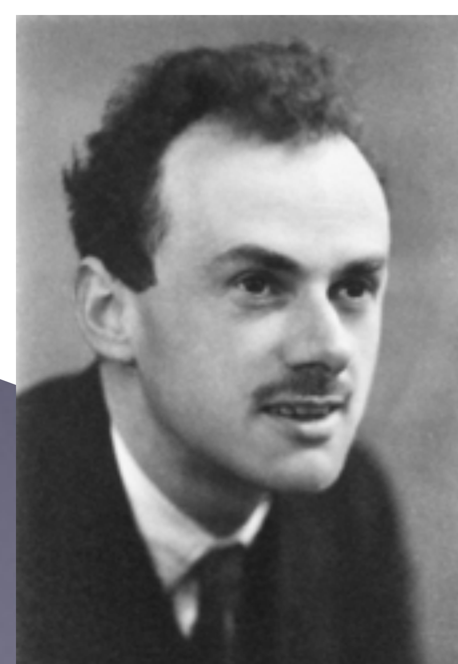
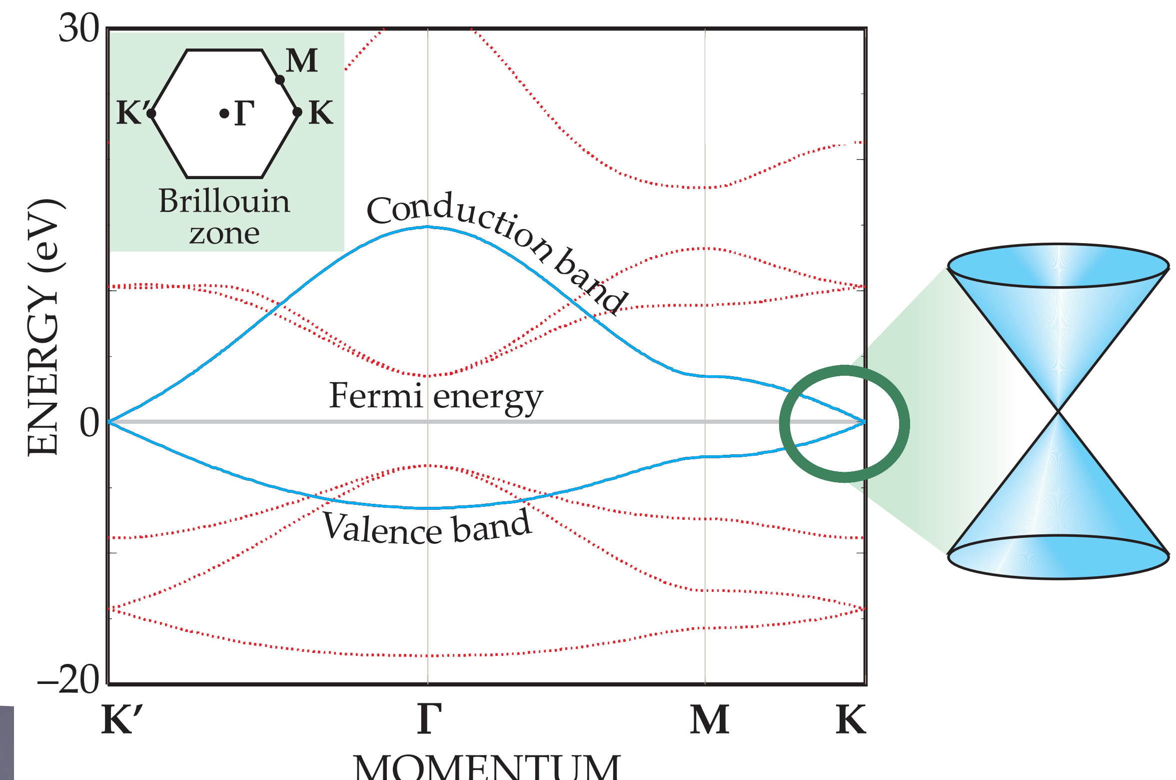
$$\hat{h} = \frac{1}{2}\boldsymbol{\sigma}\cdot\frac{\boldsymbol{p}}{|\boldsymbol{p}|} \qquad E = \hbar v_F\sqrt{k_x^2 + k_y^2}$$

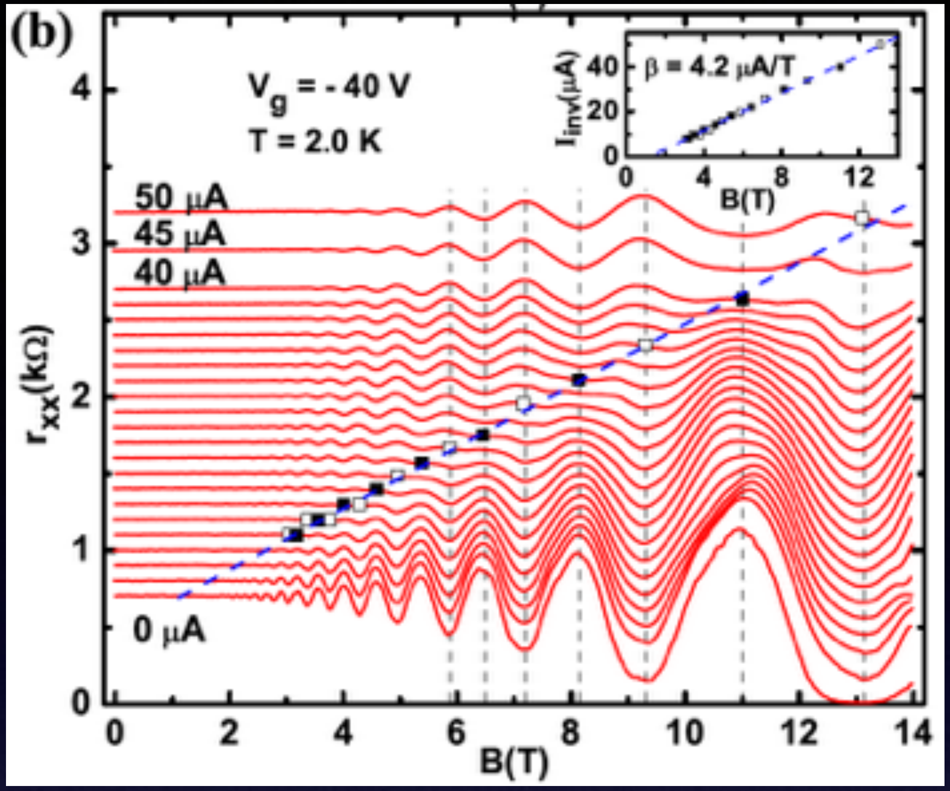
$$\hat{h}\psi_{\boldsymbol{K}}(\boldsymbol{r}) = \pm\tfrac{1}{2}\psi_{\boldsymbol{K}}(\boldsymbol{r})$$



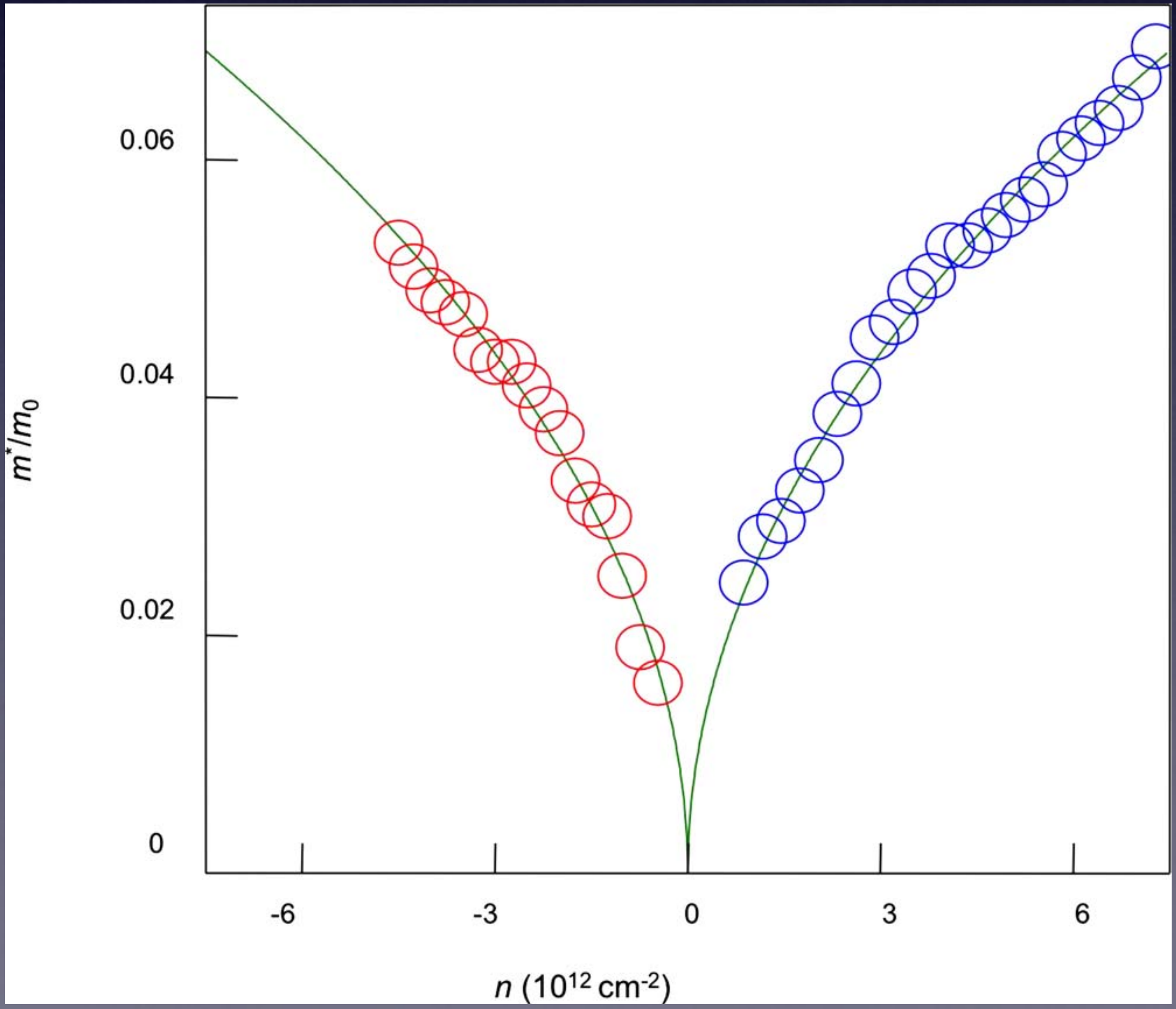




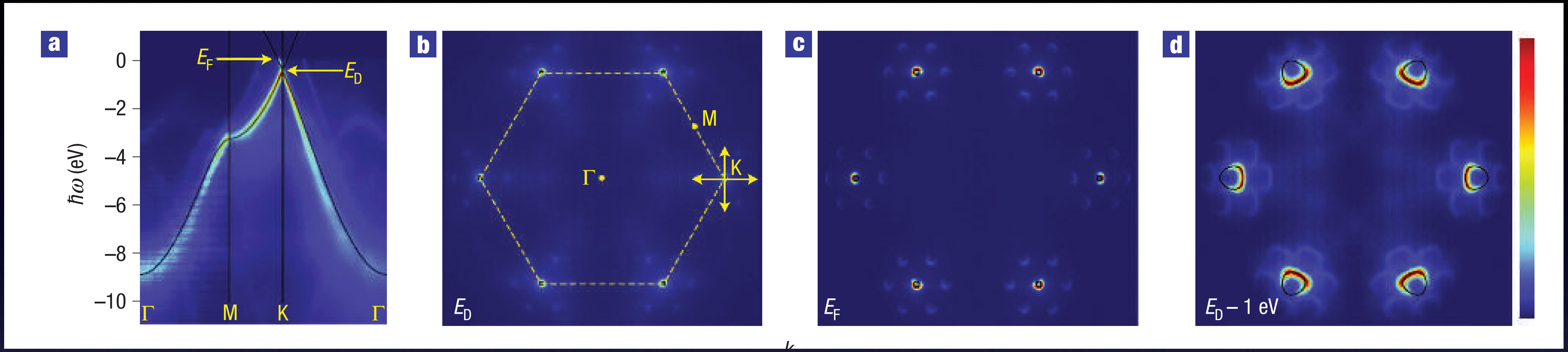
Cyclotron mass



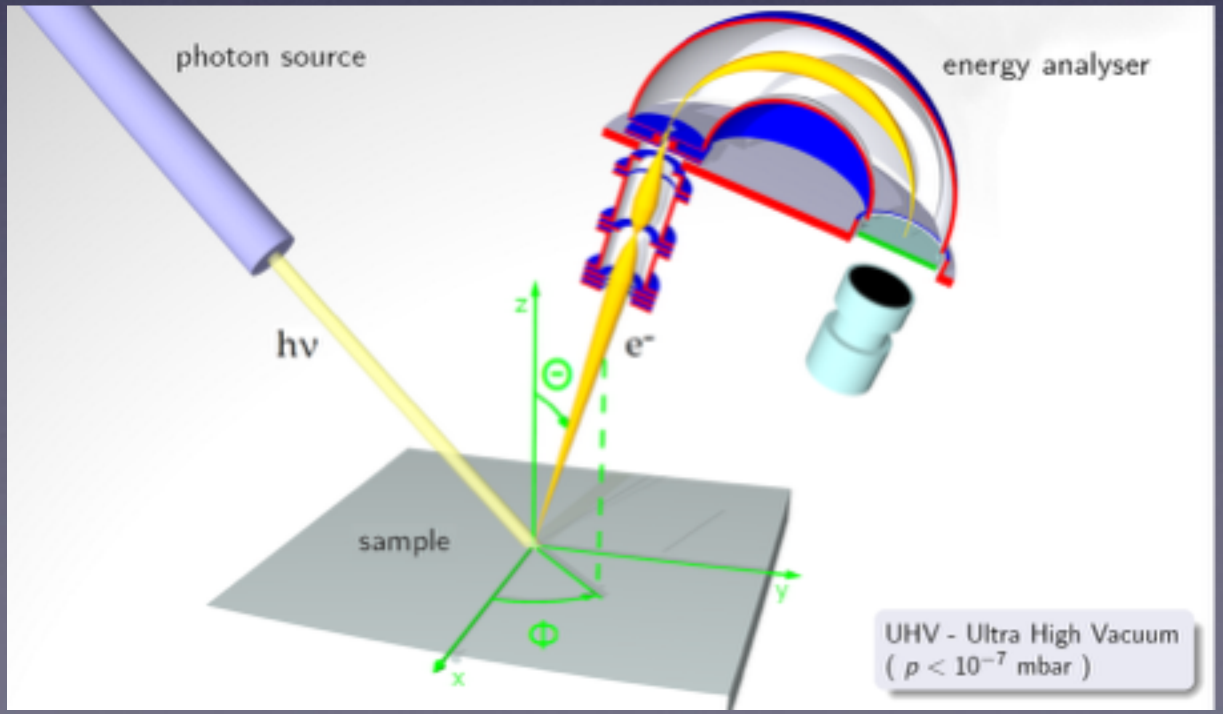
- Shubnikov-de Haas oscillations (resistivity vs magnetic field)
- Doped graphene, low temperature, high magnetic fields

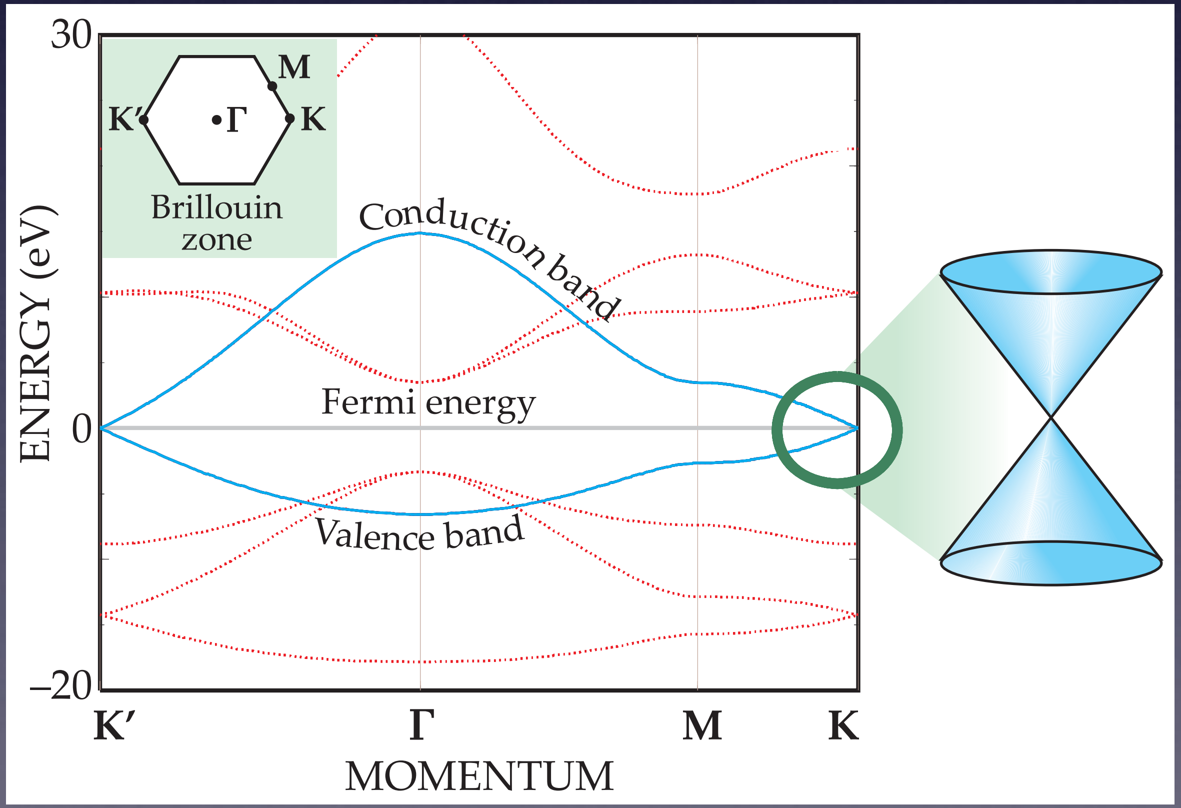


ARPES



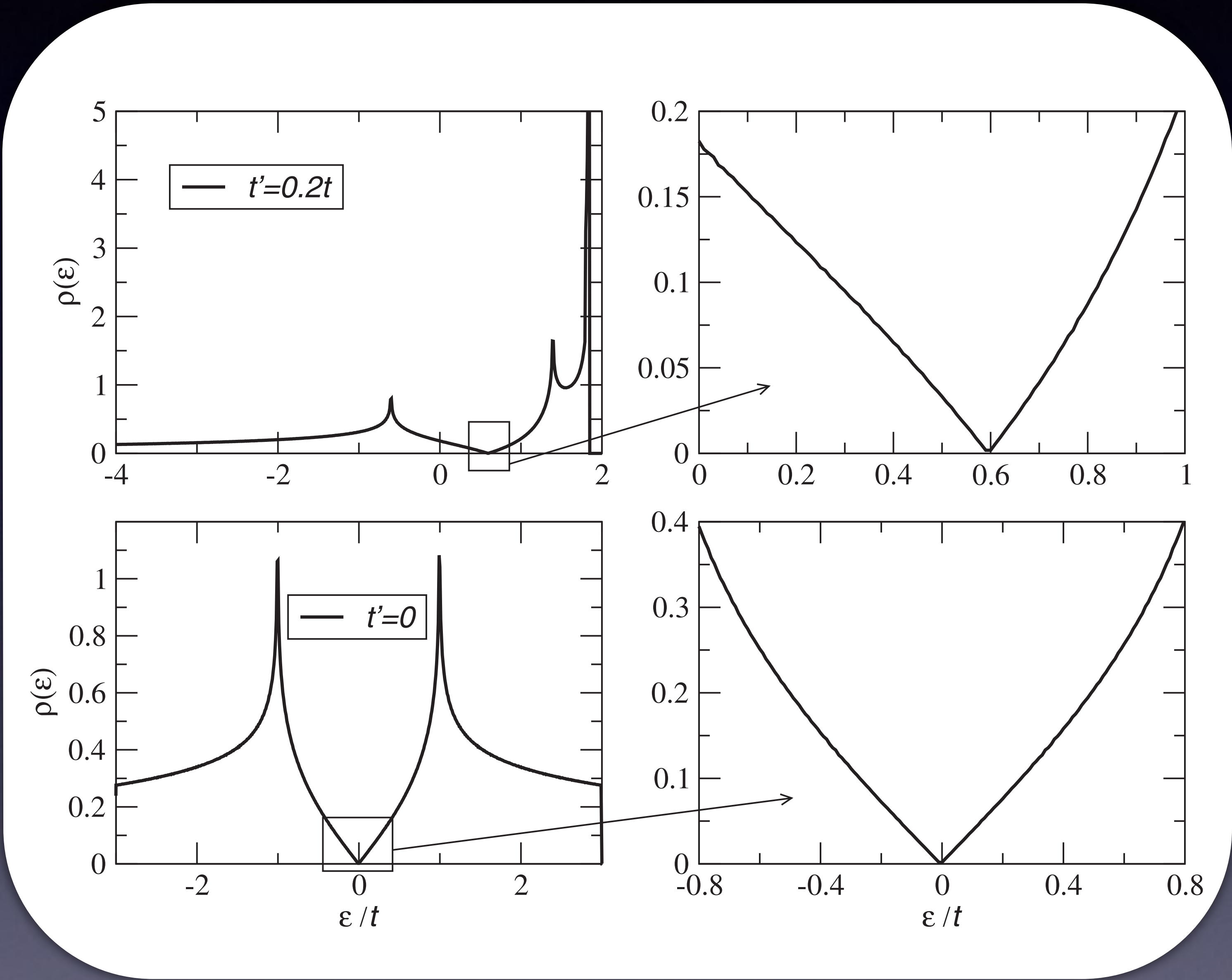
- Angle resolved photoemission spectroscopy (ARPES)



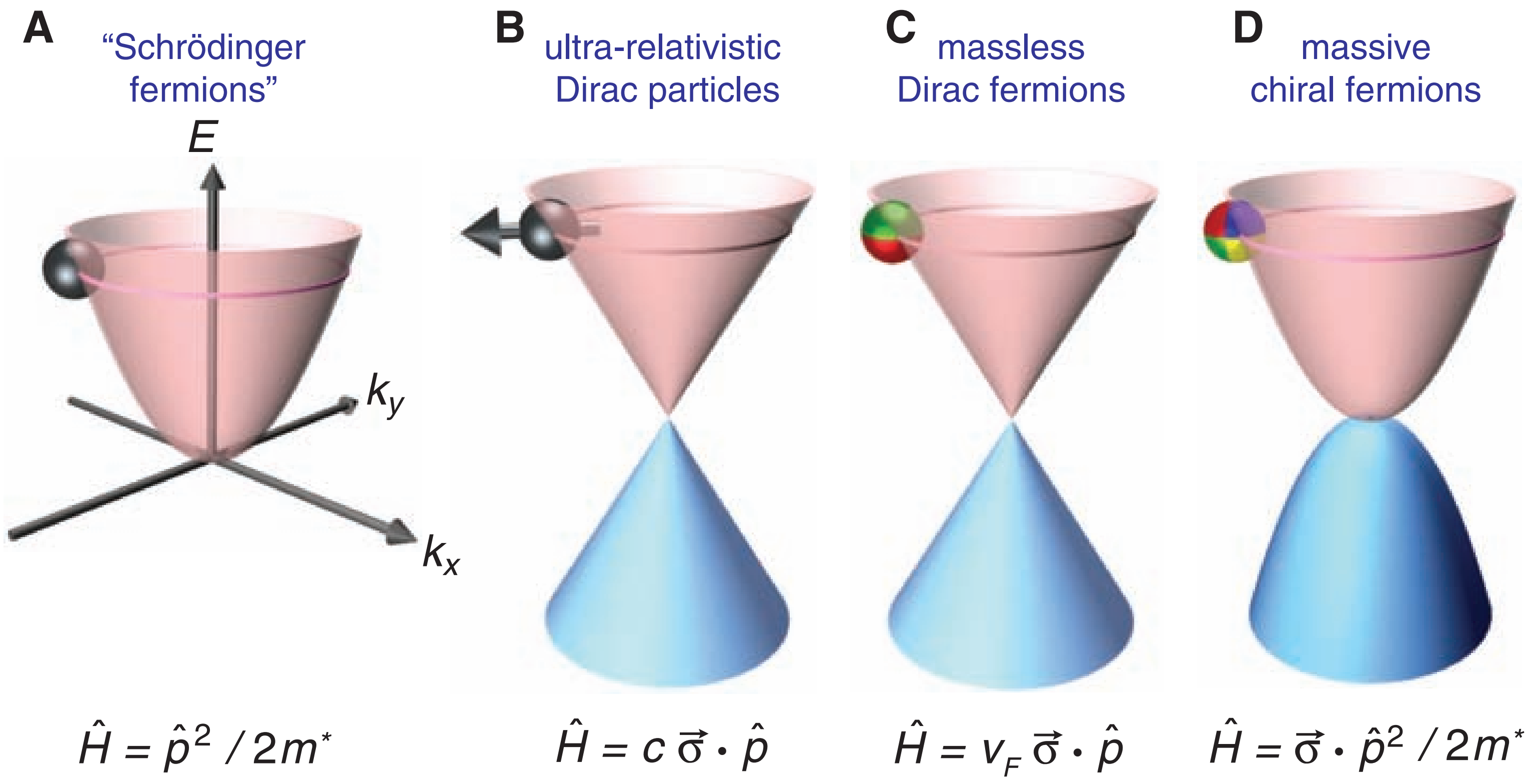


Graphene D.O.S.

- DOS is zero at the Dirac point and grows linearly
- Van-Hove singularities in the deep UV
- Linear dispersion works up to around 400 nm wavelength
- Matrix element (dipole moment) is the *exact inverse* of the DOS

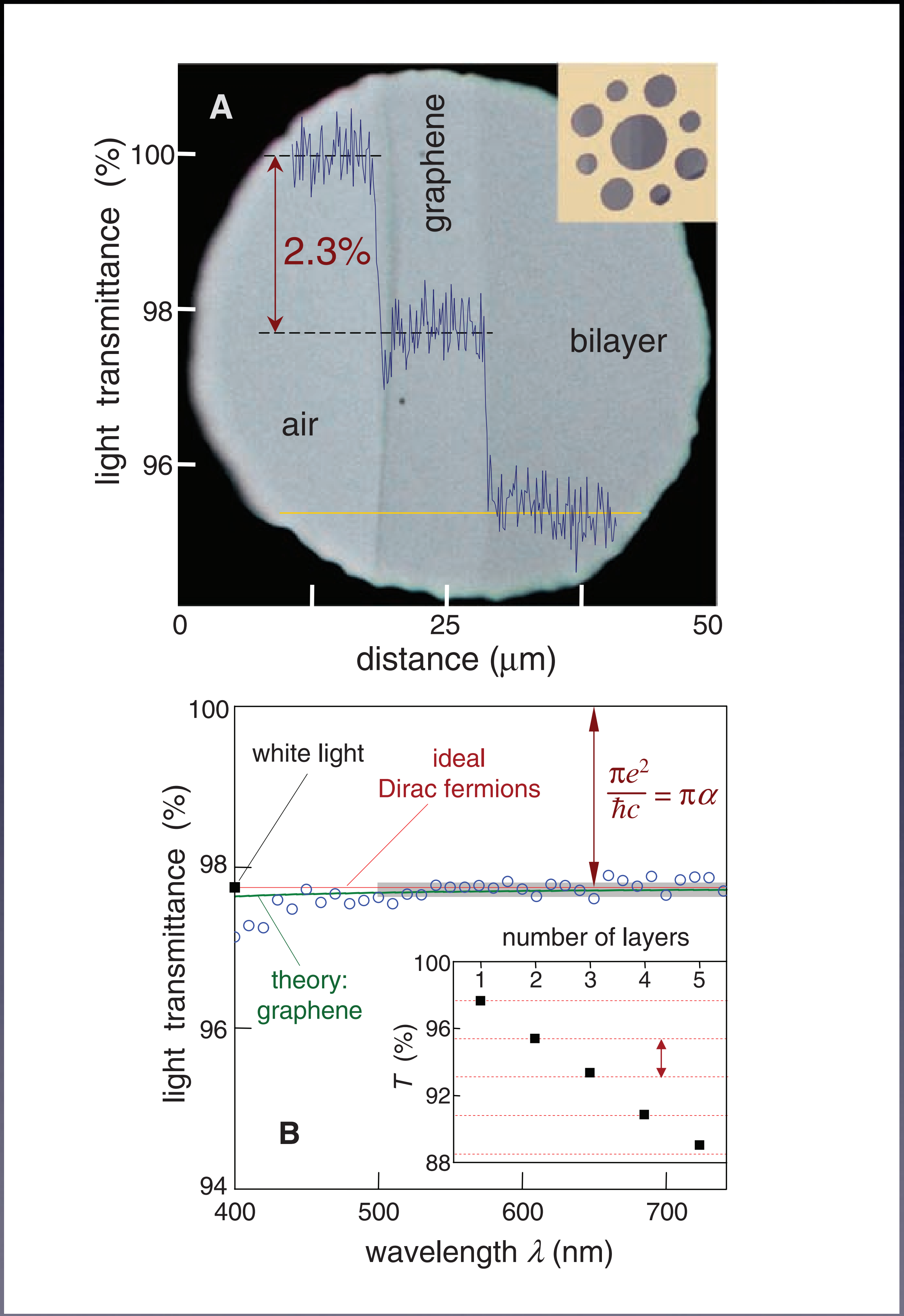


Several types of fermions in CMP



Incredible property: universal absorption

- Linear property (low fields)
- 2.3 % of light is absorbed by only 1 layer
- layers can be seen by naked eye
- The absorption of a single layer is largely frequency-independent, and proportional to the fine structure constant

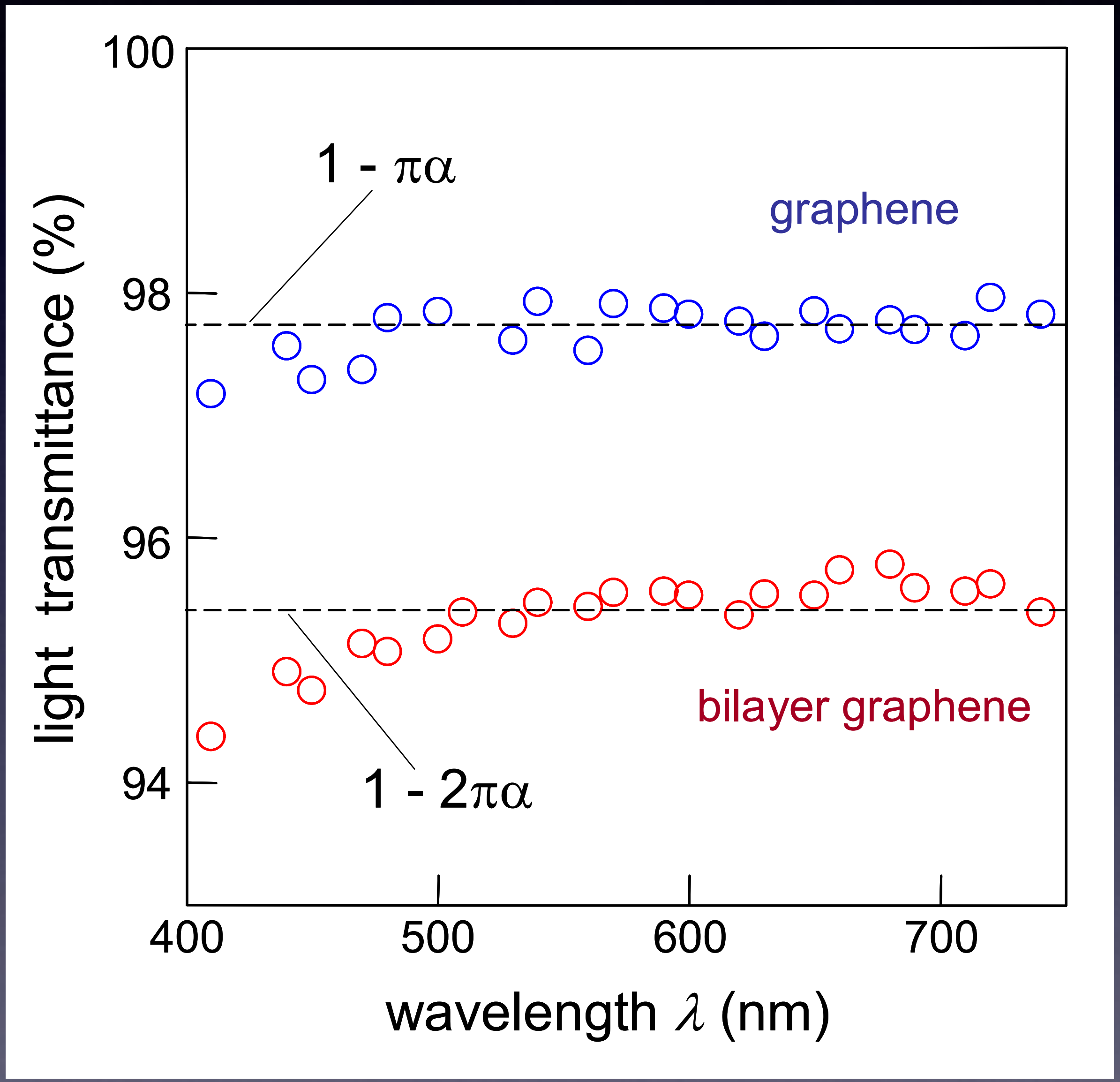


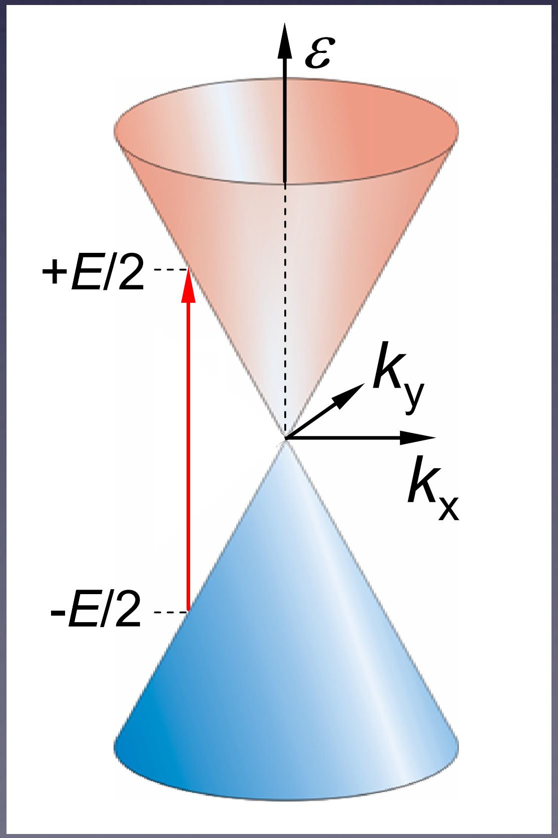
Fine Structure Constant Defines Visual Transparency of Graphene

R. R. Nair,[1] P. Blake,[1] A. N. Grigorenko,[1] K. S. Novoselov,[1] T. J. Booth,[1] T. Stauber,[2] N. M. R. Peres,[2] A. K. Geim[1]*

Monolayer and Bilayer graphene

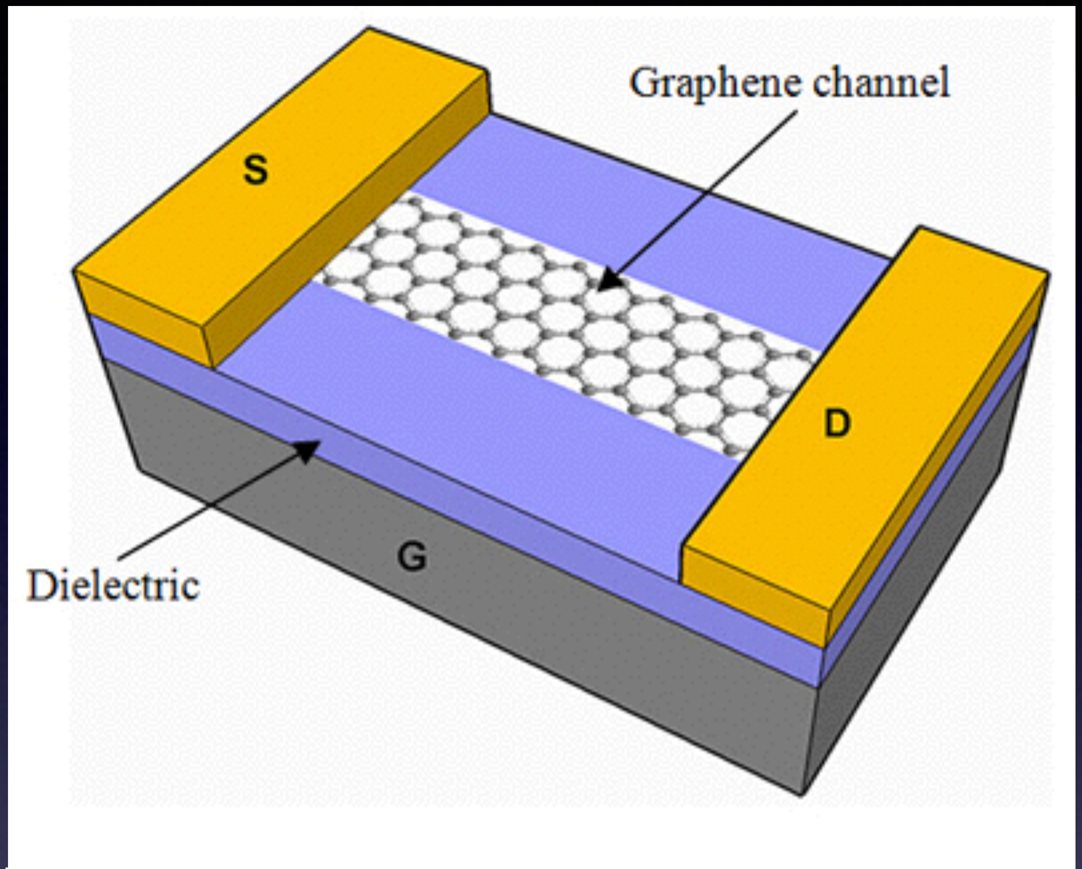
- Universal Quantum conductivity
- Law of universal absorption (linear)

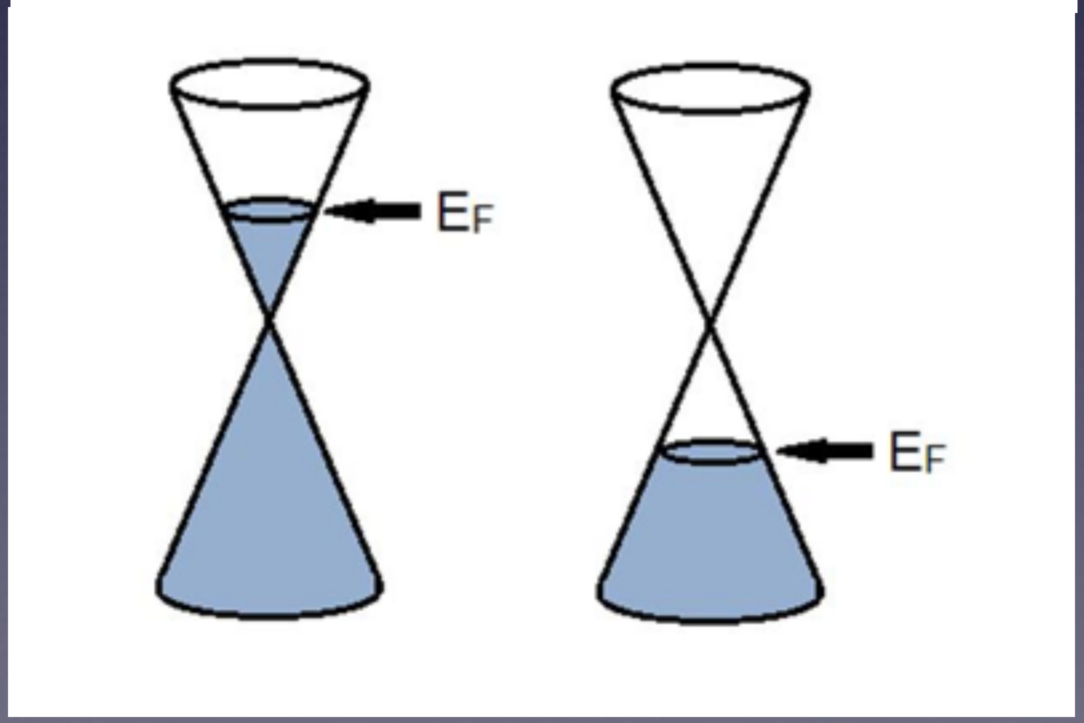




Doping graphene

- Graphene can be p-doped or n-doped
- The doping shifts the Fermi level (chemical potential)





Magnetic fields

- Magnetic fields introduce a magnetic length scale and a cyclotron frequency scale
- Dirac equation with minimal substitution

$$\ell_B = \sqrt{\frac{c}{eB}}$$

$$\omega_c = \sqrt{2}\frac{v_F}{\ell_B}$$

$$v_F[\vec{\sigma} \cdot (-i\nabla + e\mathbf{A}/c)]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

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Free electron under magnetic field

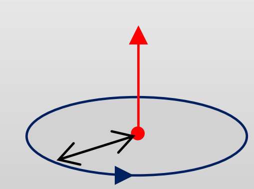
$$\tilde{H} = \frac{(\tilde{\mathrm{p}} - e\mathbf{A}/c)^2}{2m}$$

Energy and orbit are quantized:

$$\varepsilon_n = \hbar w_c(n + 1/2), \qquad w_c = eB/mc$$

Each Landau orbit contains magnetic flux quanta

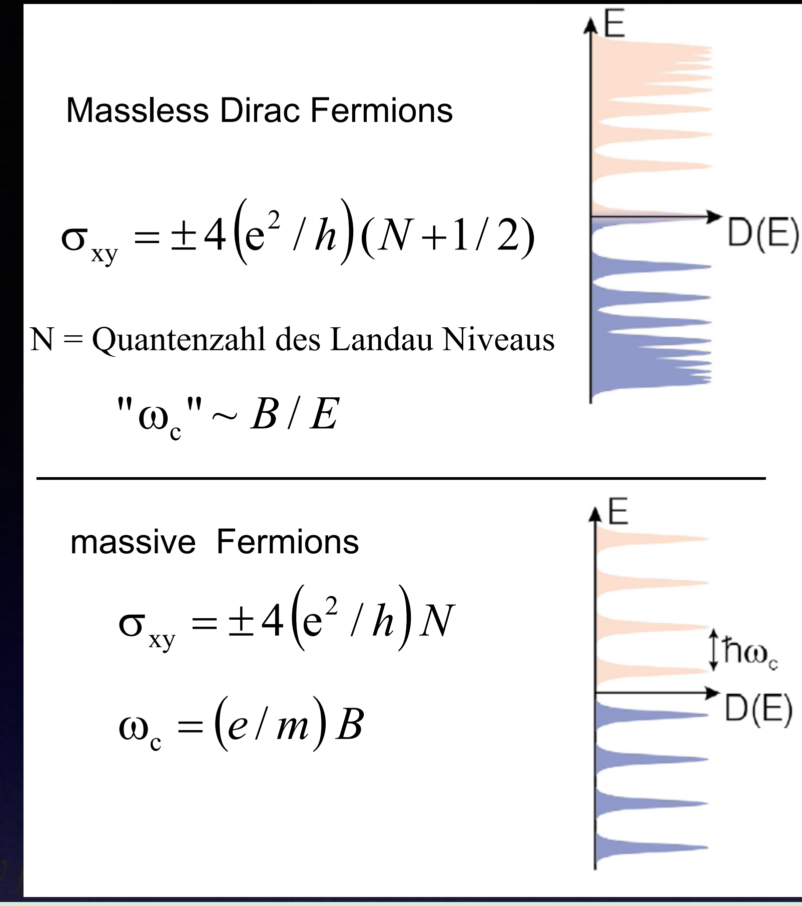
$$\phi_0 = \frac{hc}{e}$$

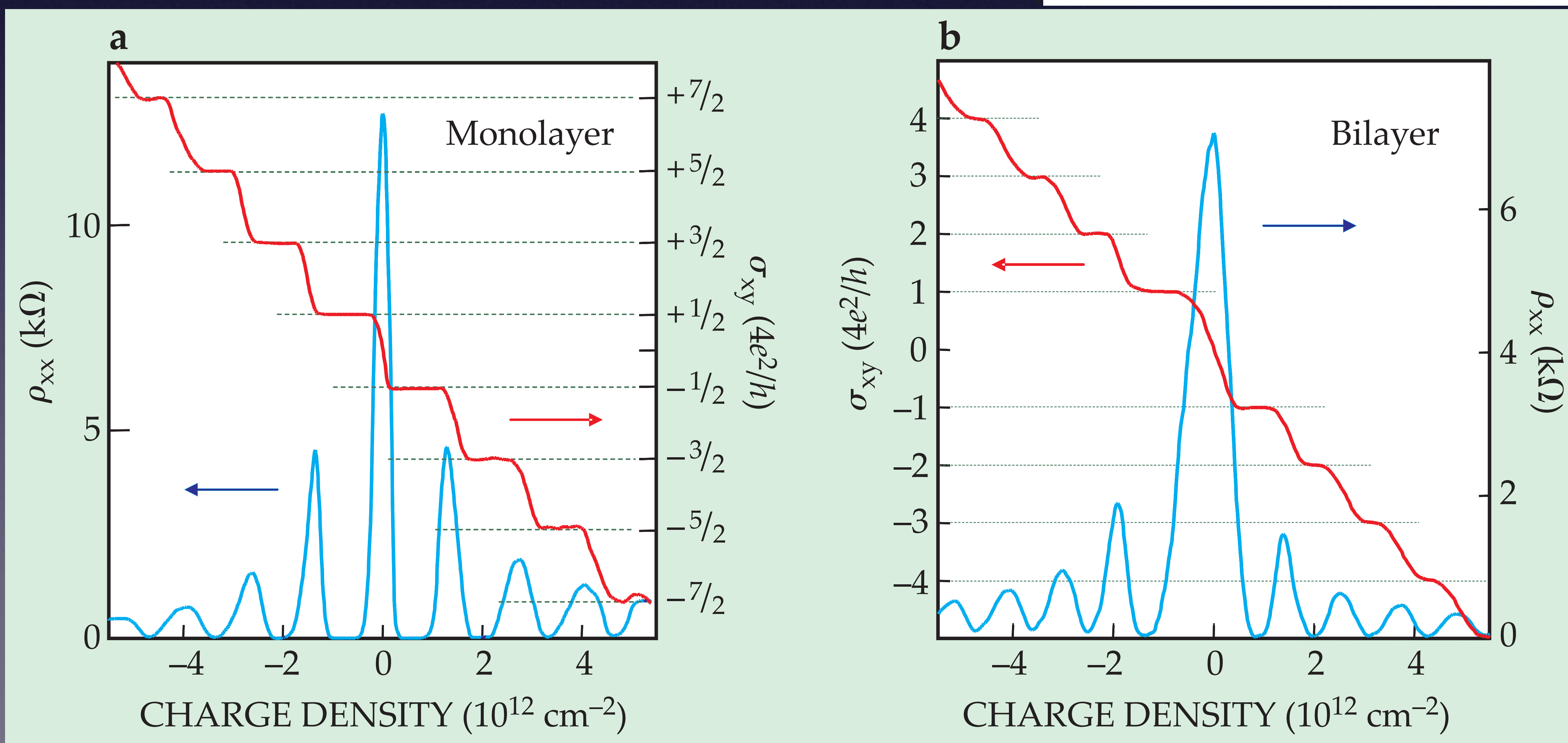


$$\ell_B = \sqrt{\hbar/eB}$$

Quantized Hall effect

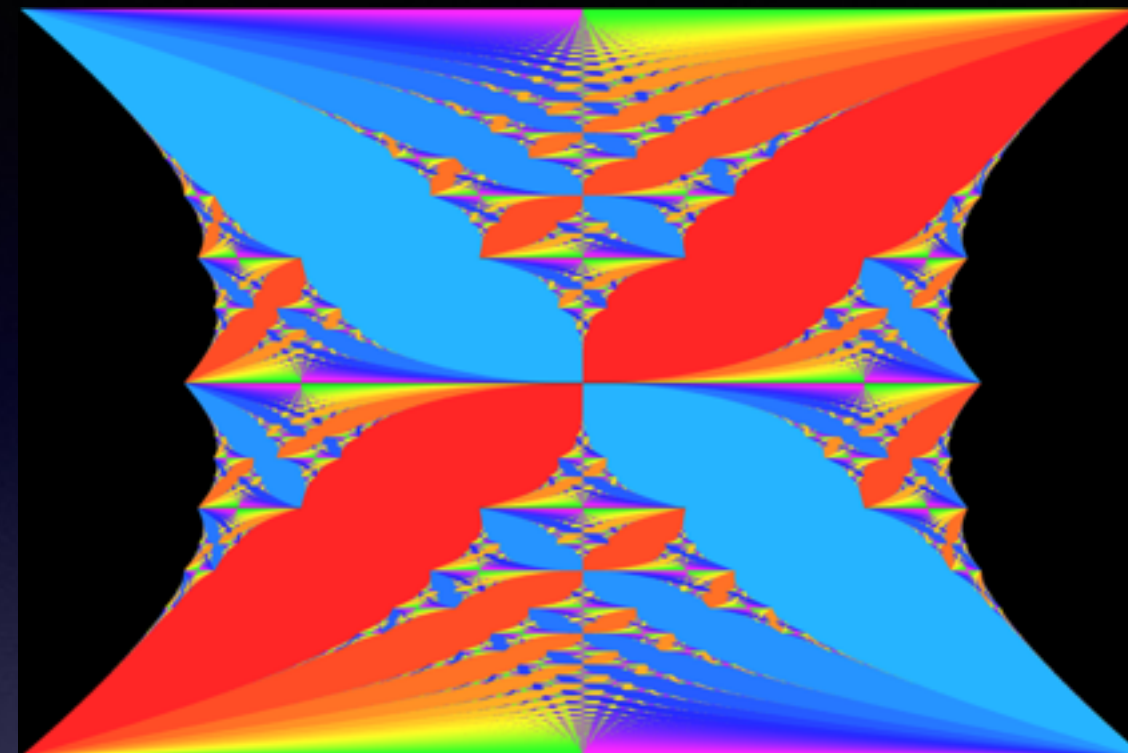
- Landau levels

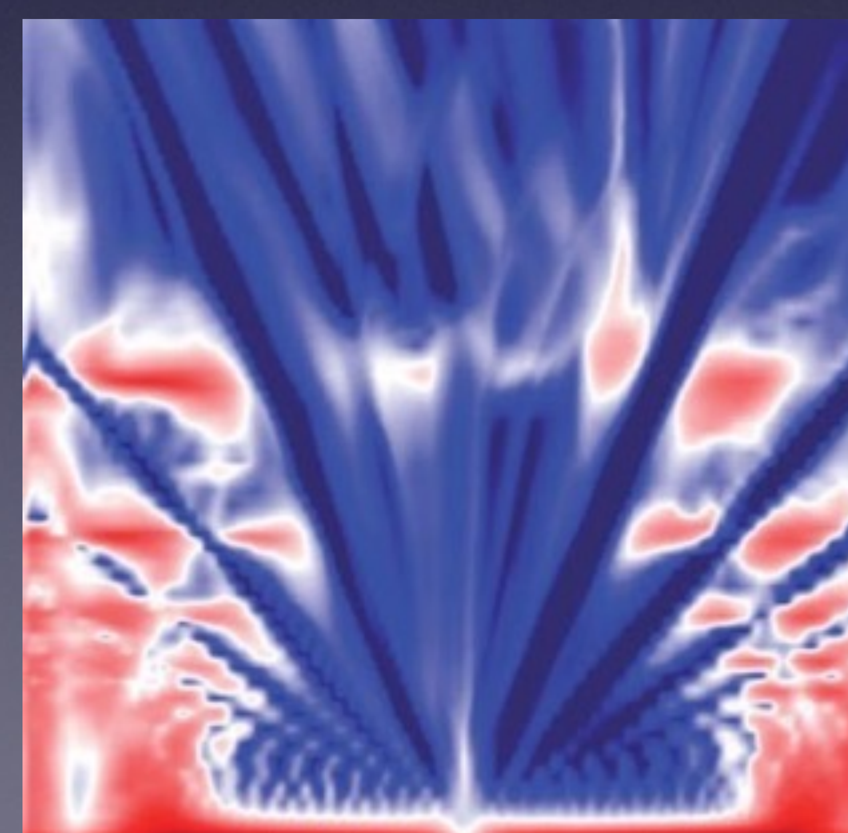




Hofstadter butterfly

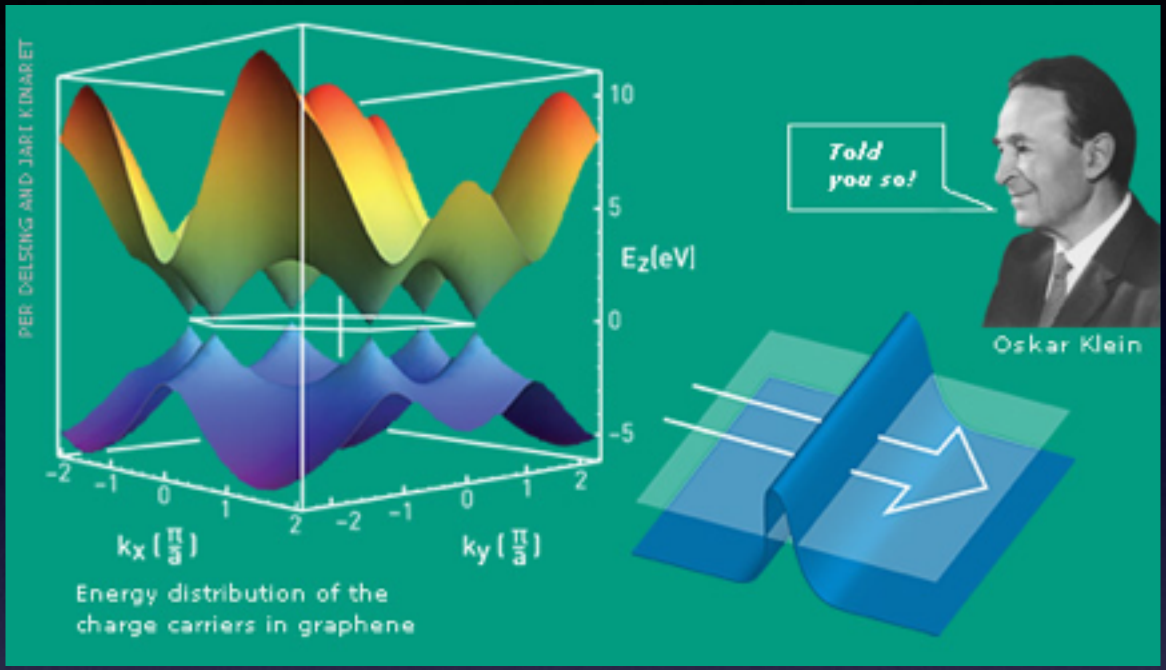
- Predicted by the cognitive scientist Douglas Hofstadter
- Chemical potential vs magnetic field
- Different colours are different integers in the quantum Hall conductance
- Warm colours are positive integers, cold colours are negative integers
- Fractal structure

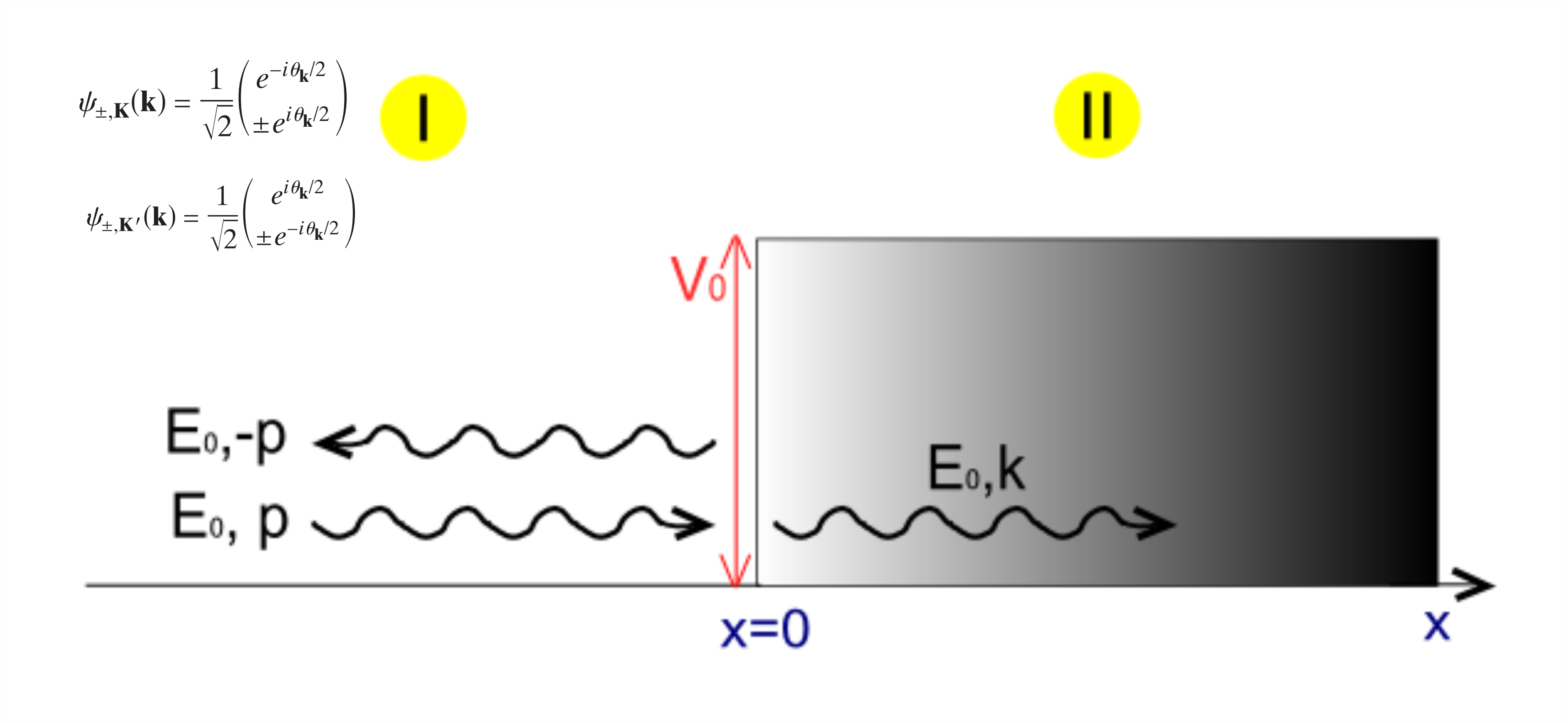




Klein paradox

- Predicted by O. Klein by using the Dirac equation
- When a potential barrier is very large, the transmitted wave function is nearly one ?!?
- The electron is transmitted as a hole in the barrier

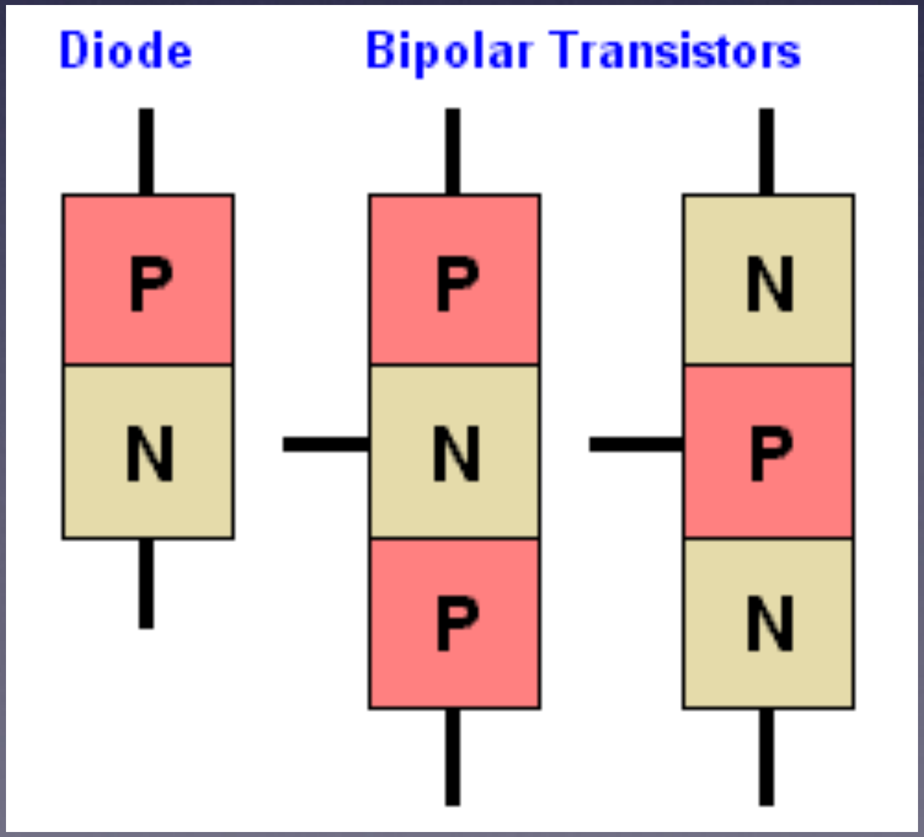




Non-resistive electronics

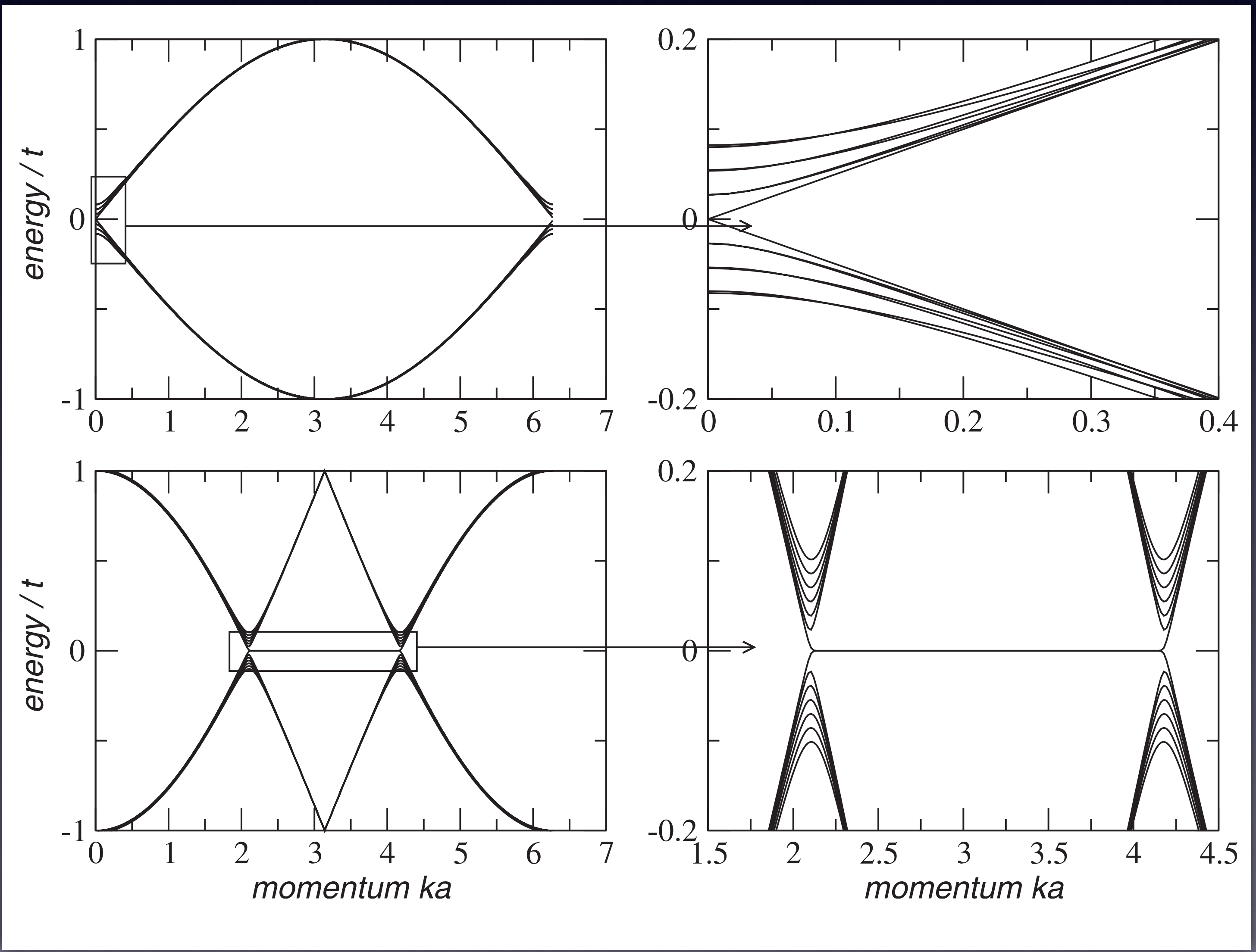
- PN junctions in ordinary diodes and transistors are non-transparent for incident electrons, therefore they are highly resistive

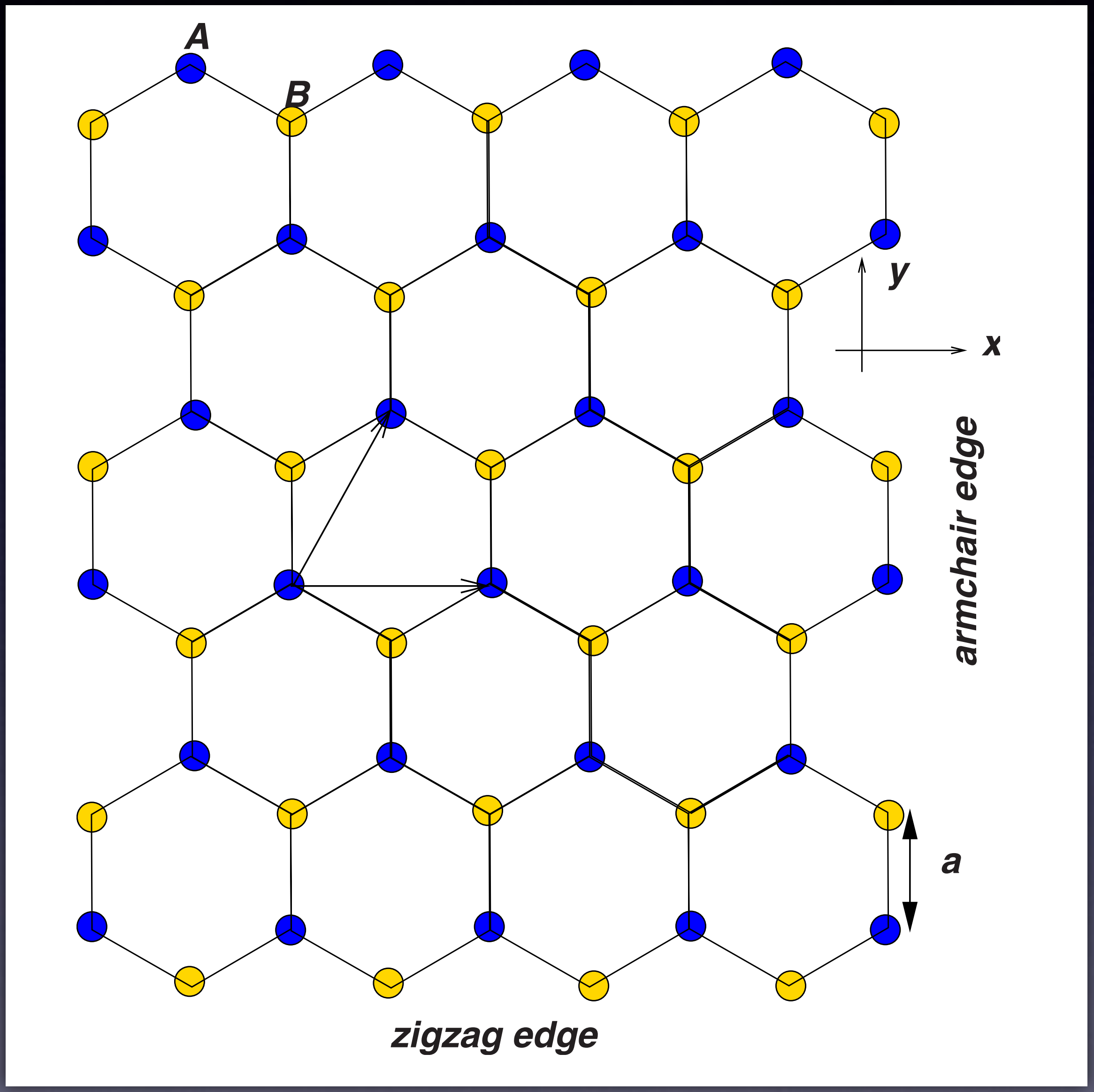
- Klein paradox makes the junction very transparent !



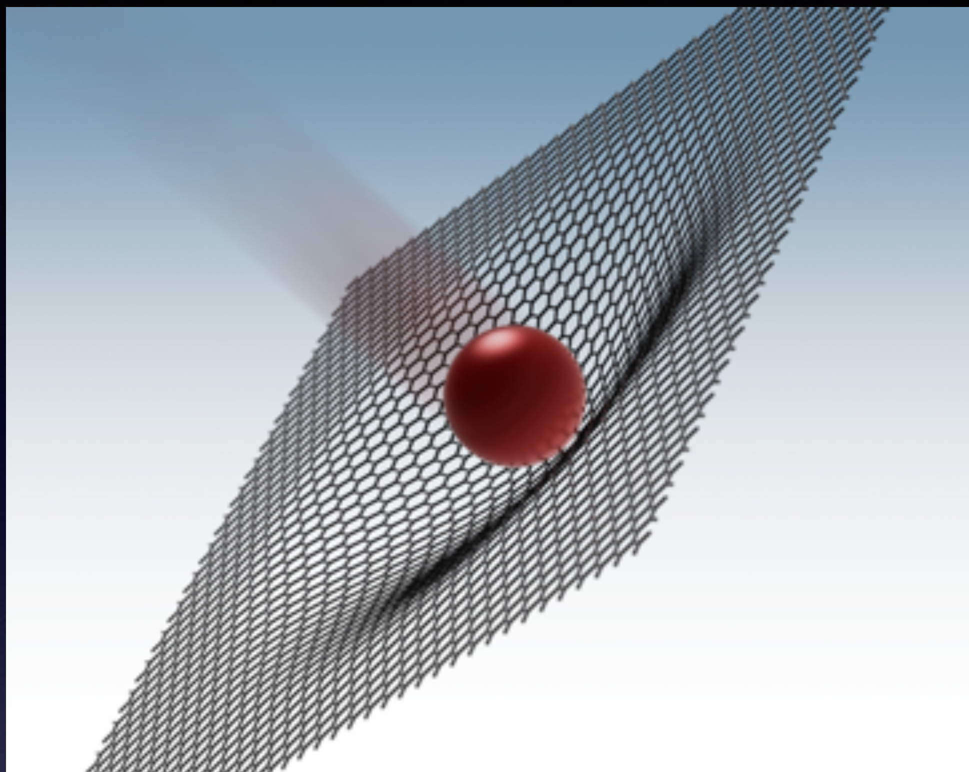
Graphene surface states

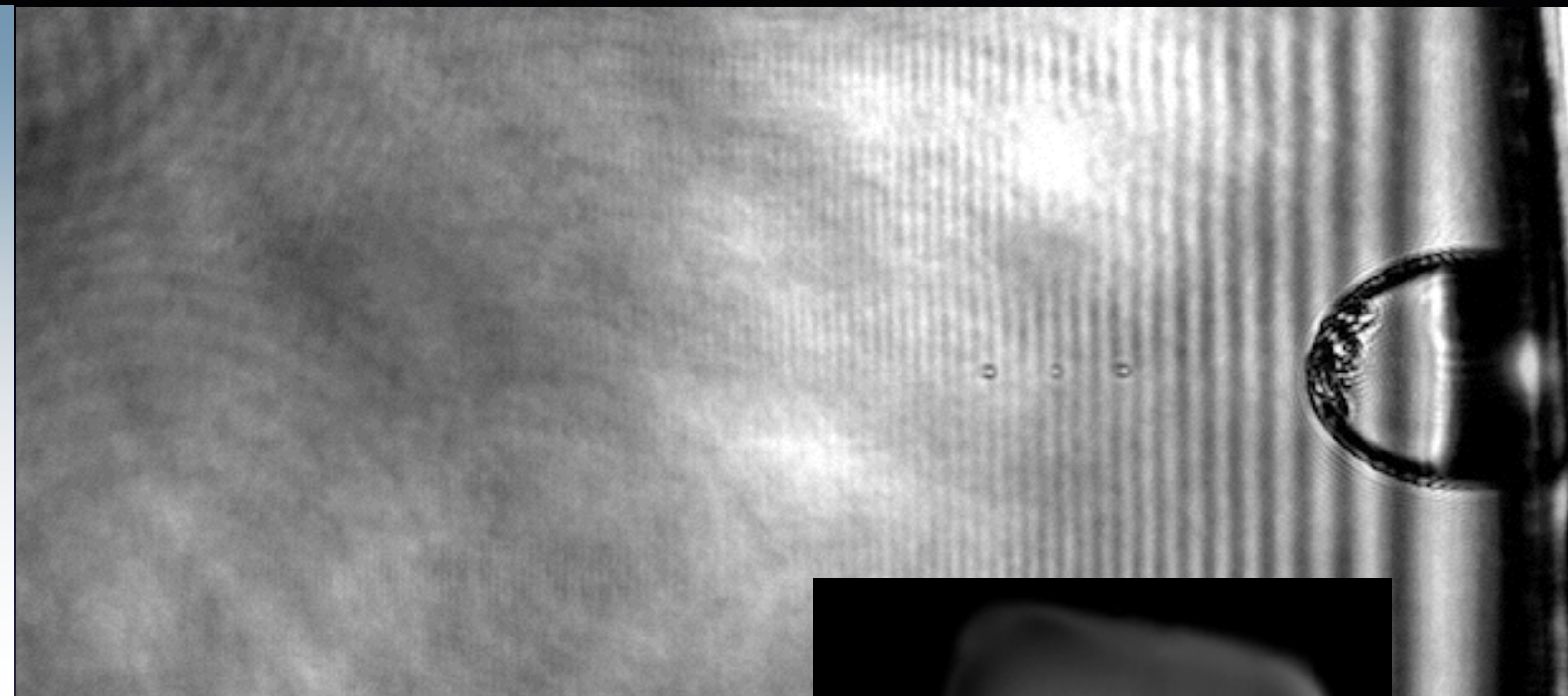
- Surface states exist when edges appear and translational symmetry is broken
- Important for the field of topological insulators

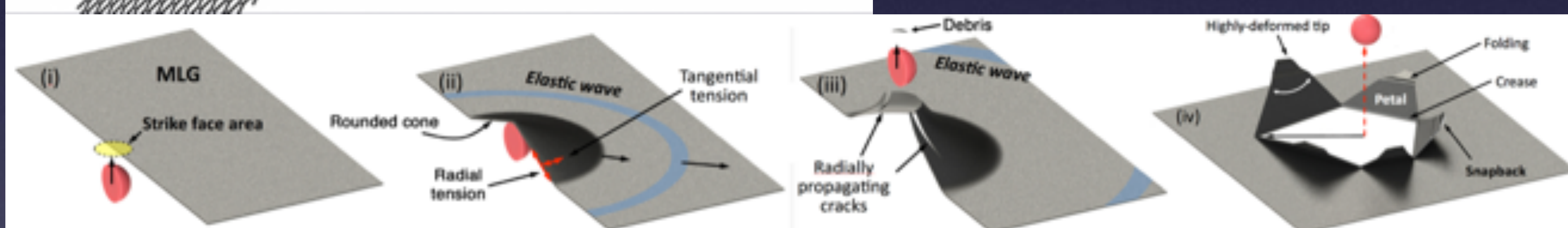


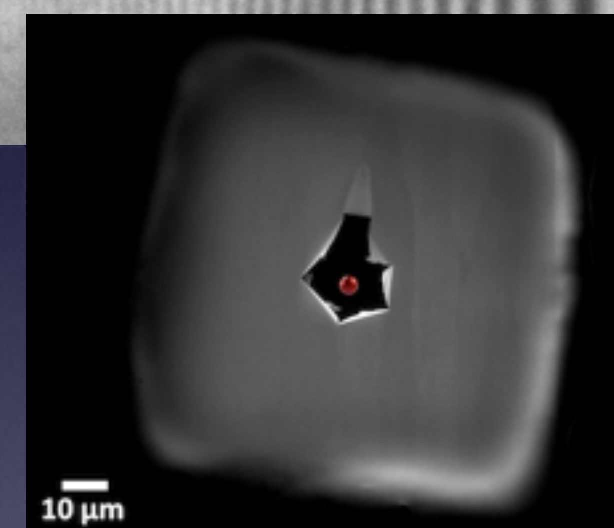


Stronger than steel

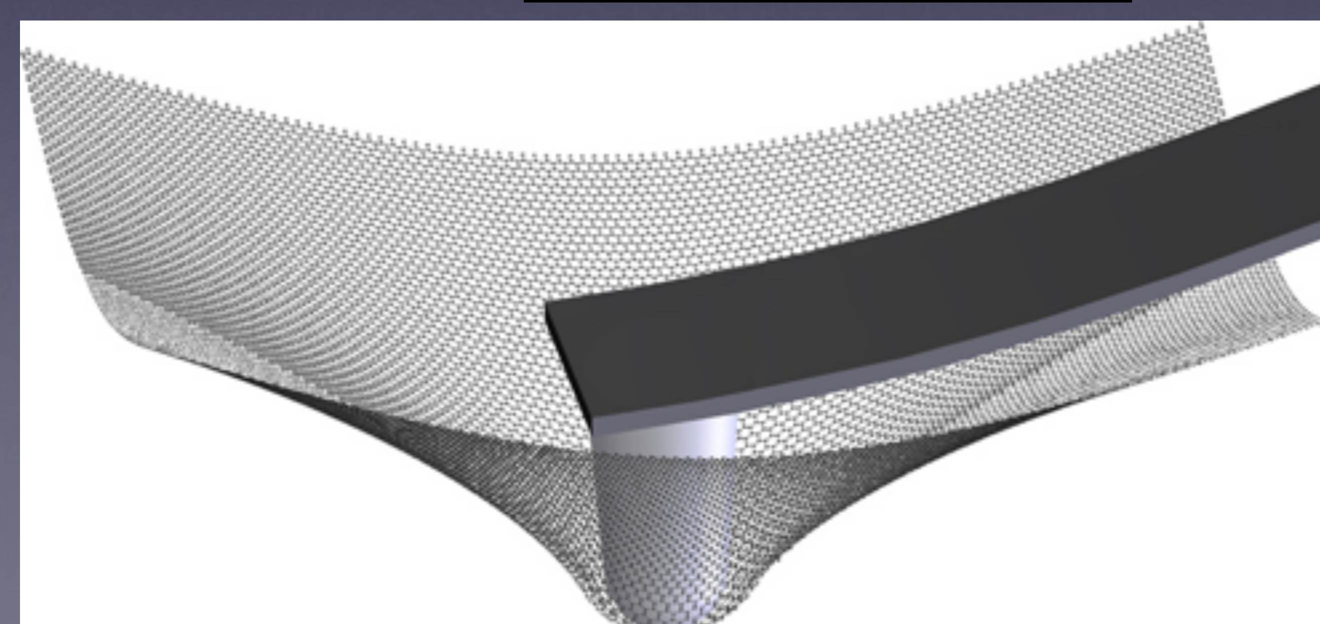






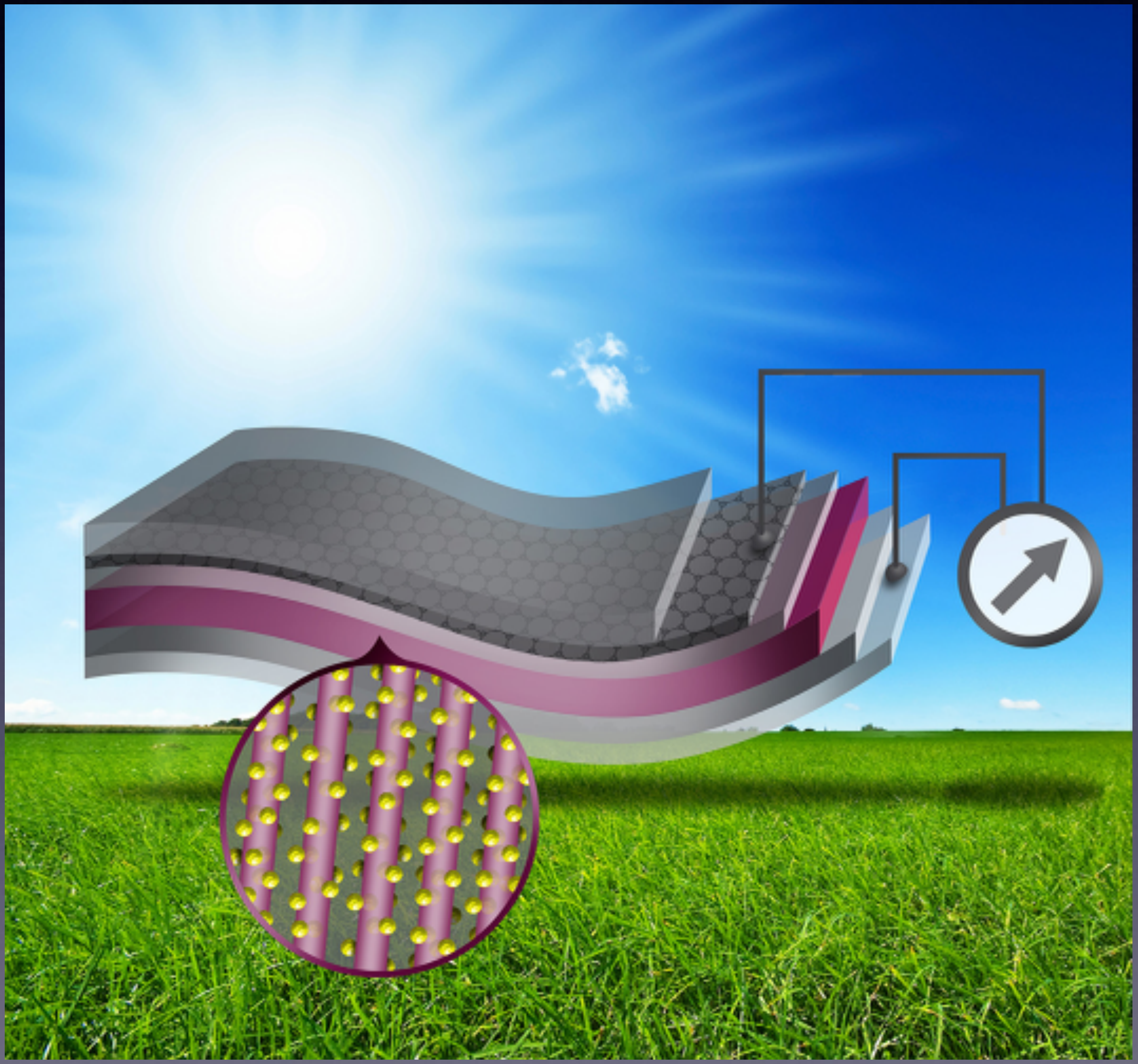


- 10 times stronger than steel
- Microbullets fired at a layer
- strength tested with mechanical tips



Graphene solar cells

- graphene is a “transparent conductor”
- ideal for solar cells
- silicon cells efficiency is around 30%
- graphene-silicon cells could reach a 60% efficiency

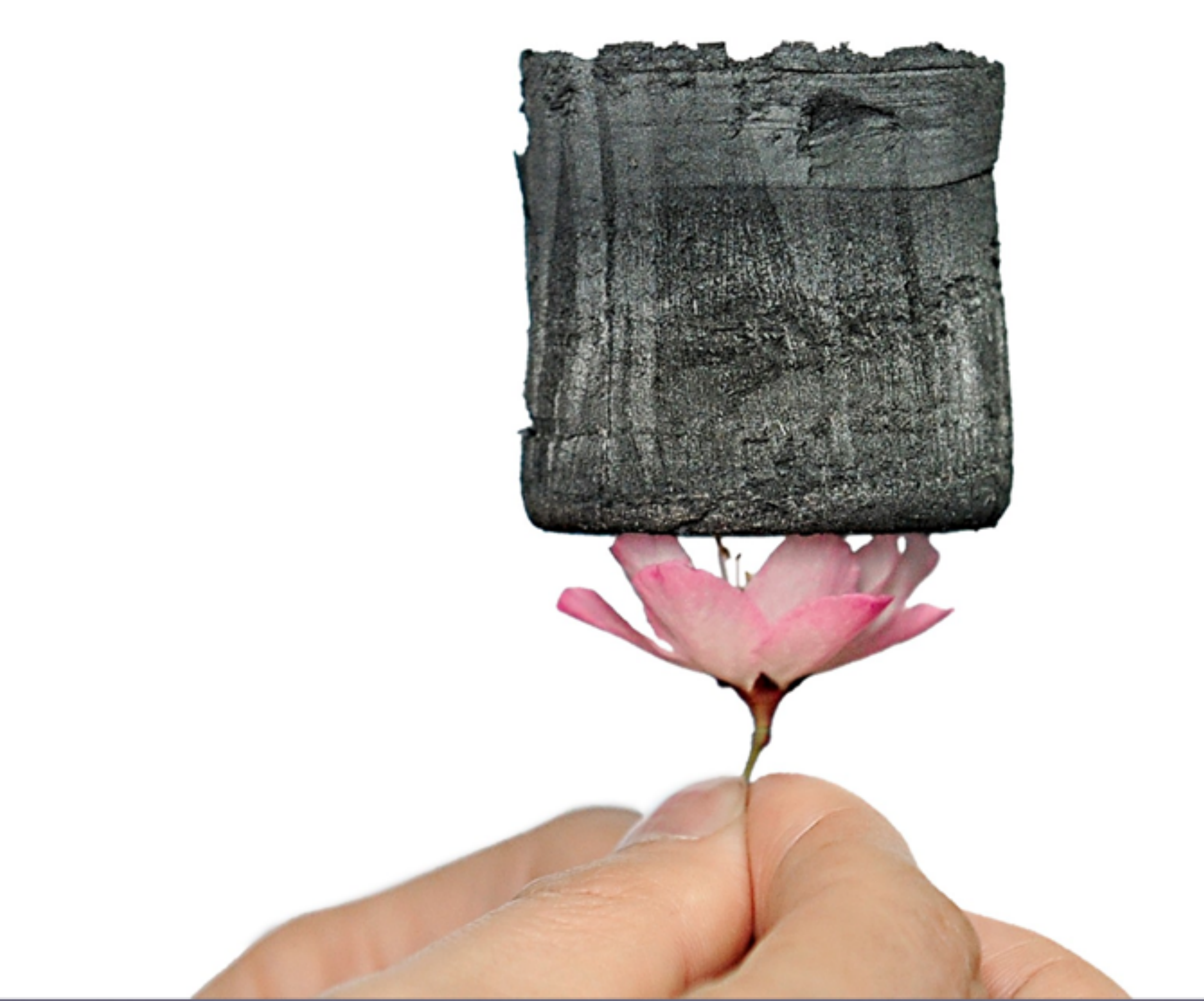


Graphene light bulbs

- Last 10% longer than LEDs
- On sale this year (expect a Christmas present)

Graphene aerogel

- The lightest solid material in existence
- Made of graphene and carbon nanotubes
- Seven times lighter than air



Flexible graphene displays

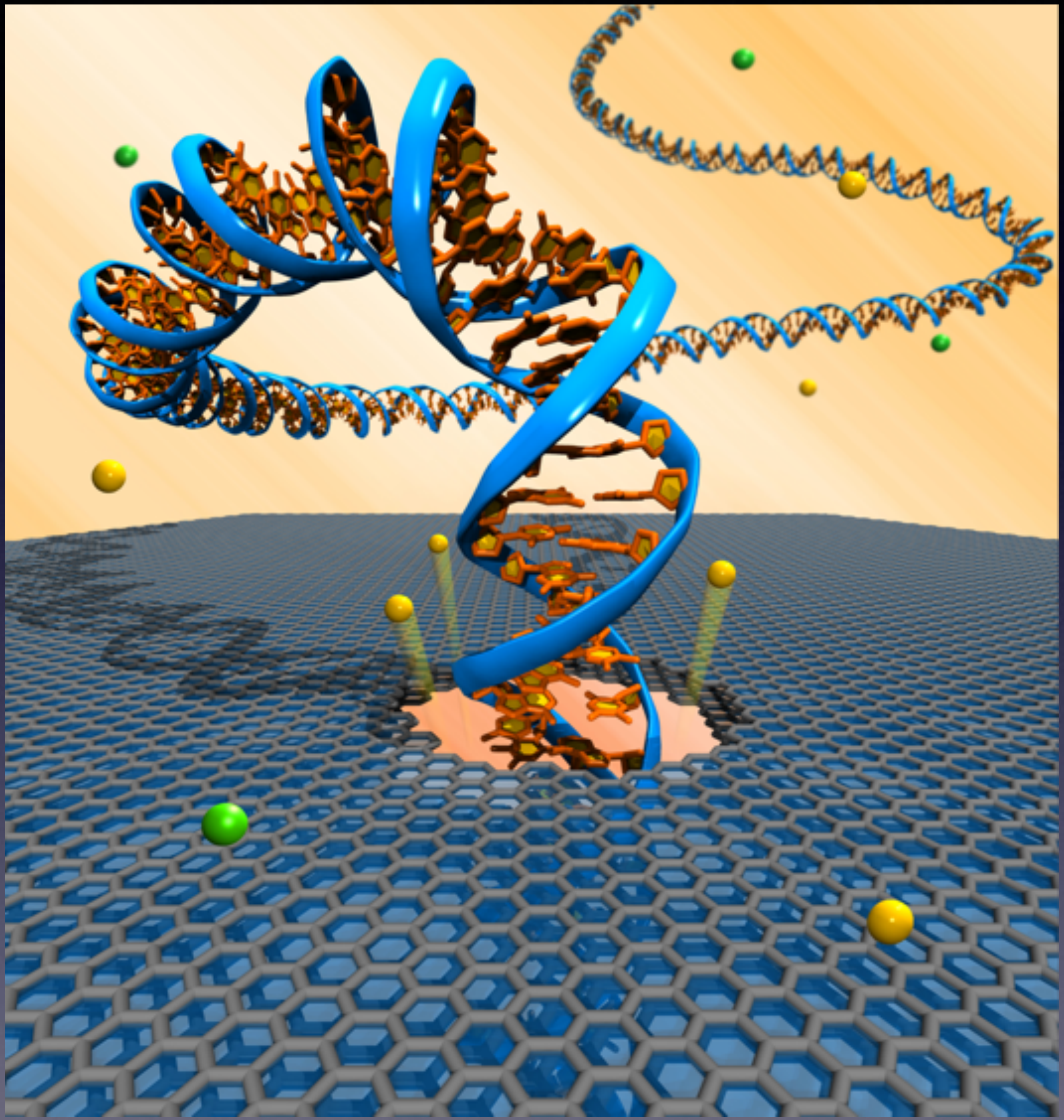
- Samsung is developing some secret projects

Vantablack

- Darkest material, absorbs 99.965 % of light in the visible
- Made of grown carbon nanotubes
- Light is continuously deflected and converted into heat, and is never reflected
- Will be used in telescopes to increase their sensitivity to faint stars

Electronic DNA sequencing

- Electrical detection of single DNA molecules
- Electric fields push DNA down a hole
- Ultimately (they say in 2030), it will be possible to sequencing DNA electronically

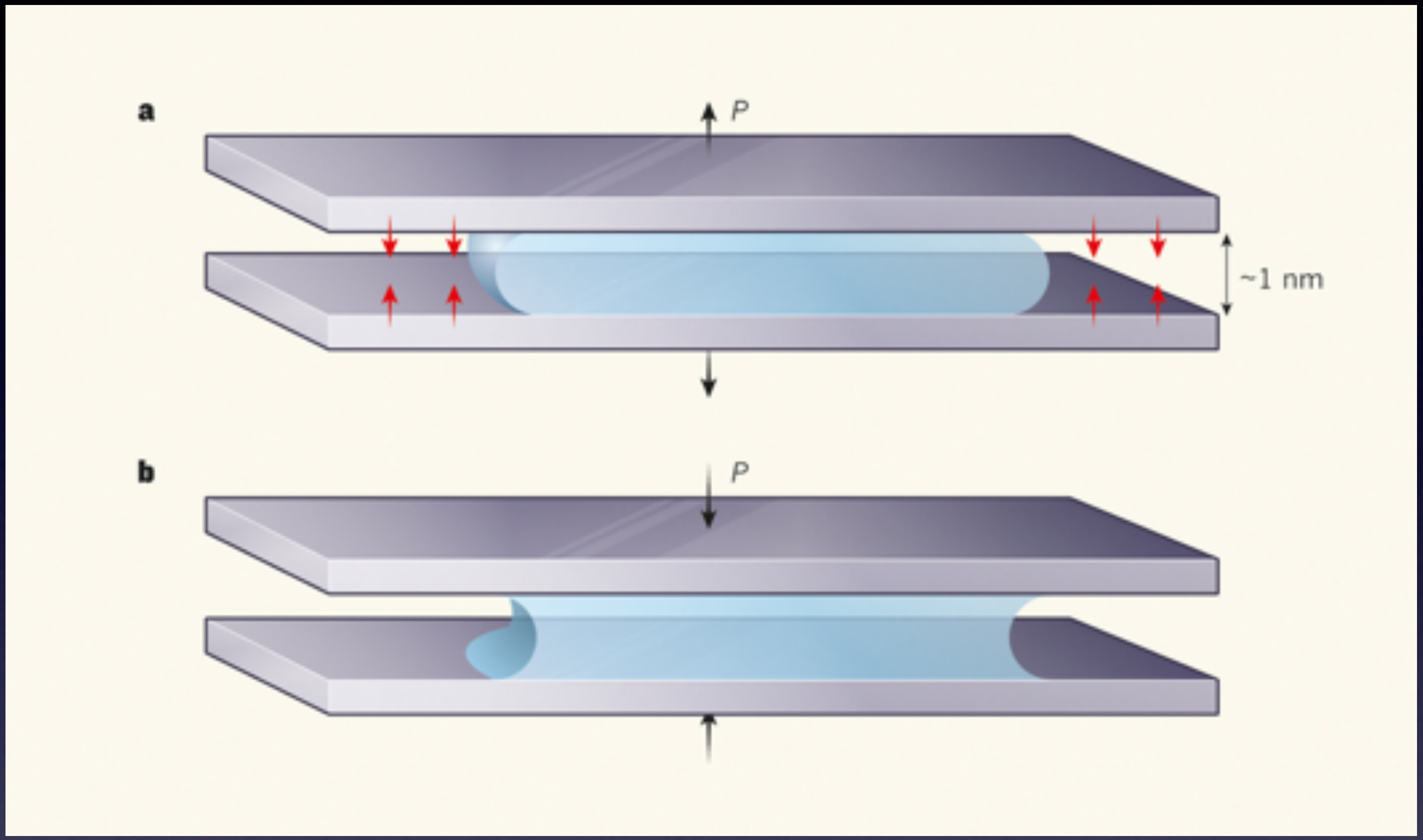


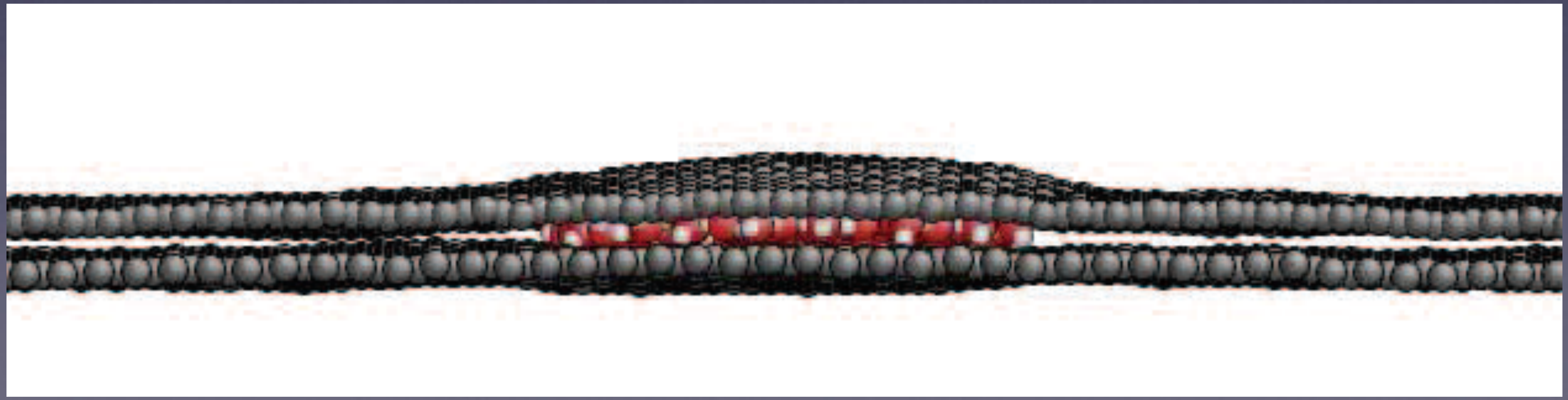
Graphene spiders

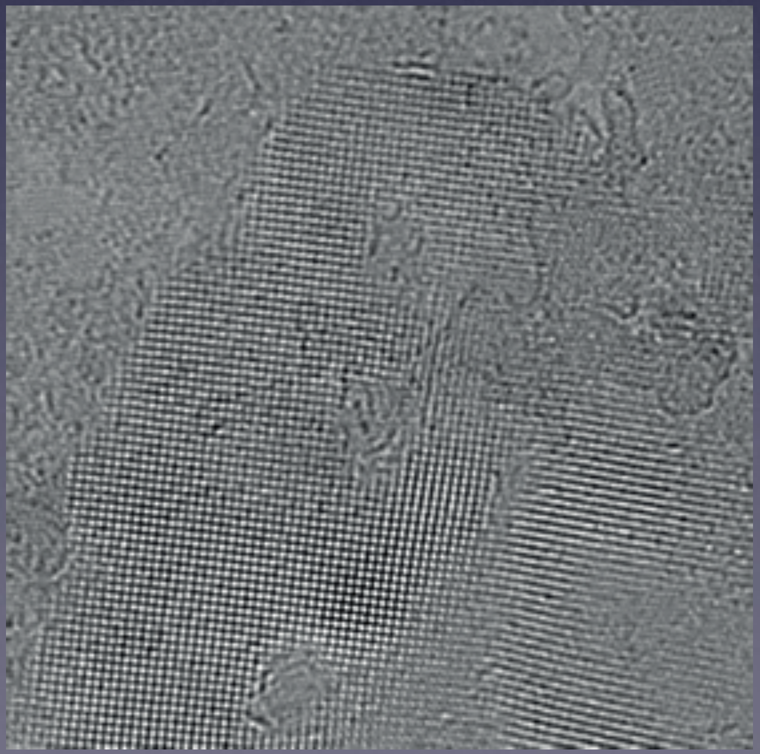
- Spiders sprayed with graphene produce super-strong silk
- A web made like this can catch a falling plane
- Candidate for the Ig-Nobel prize ?

Graphene 2D ice

- Square ice in a graphene sandwich
- Graphene ice cream?

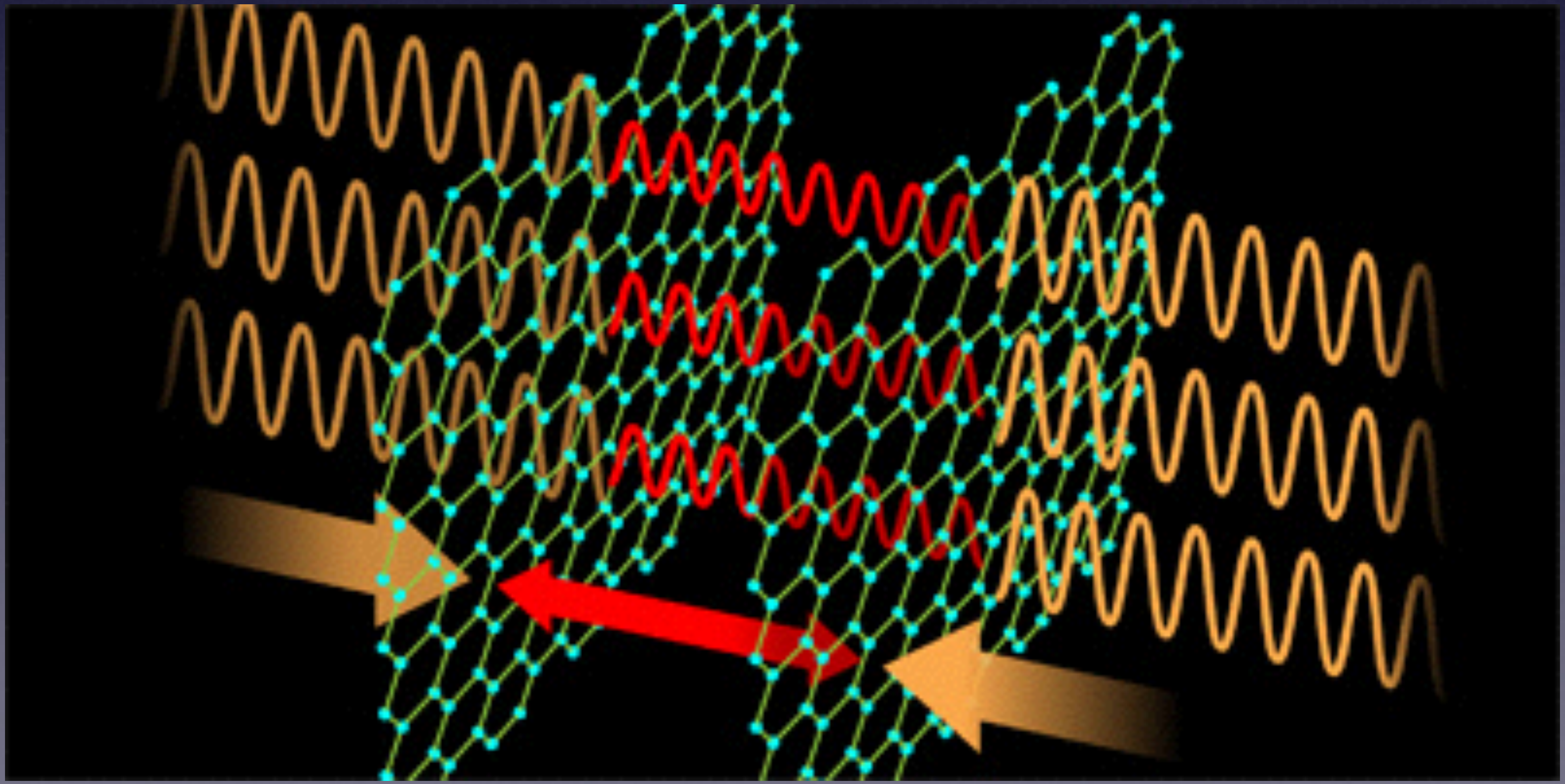






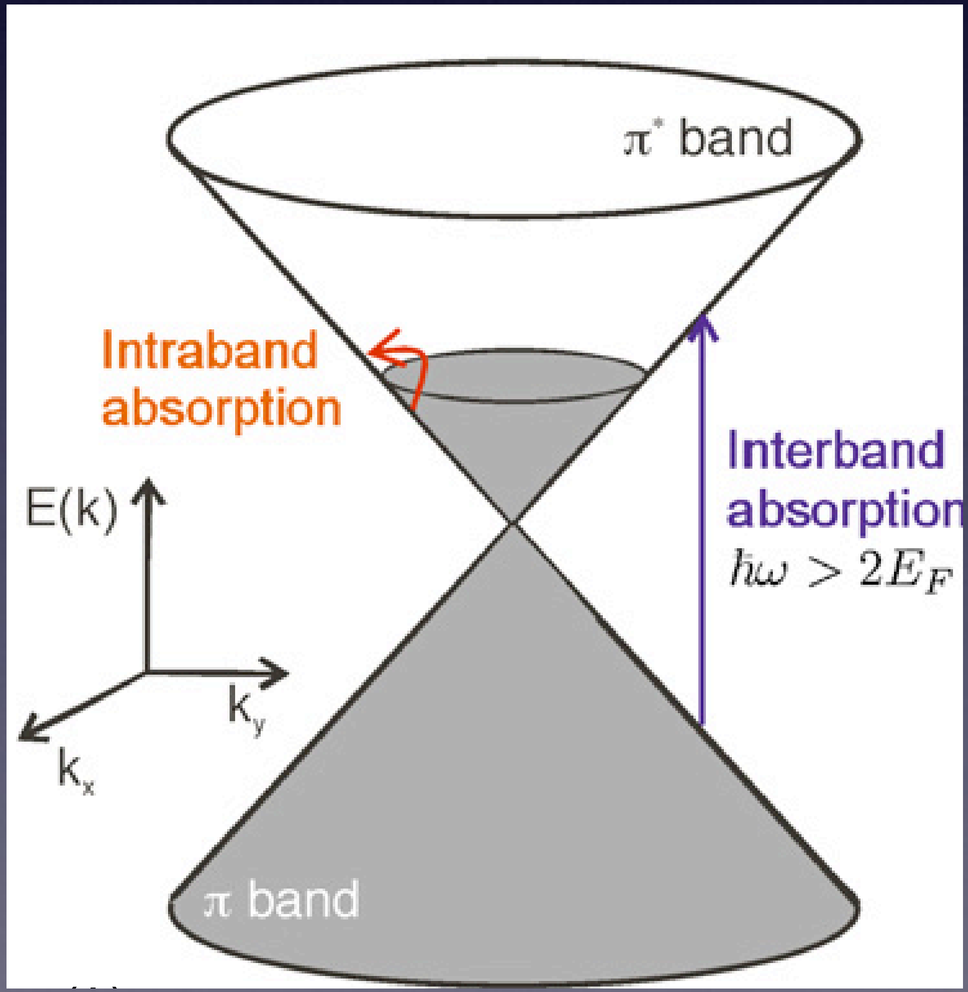
Casimir effect in graphene

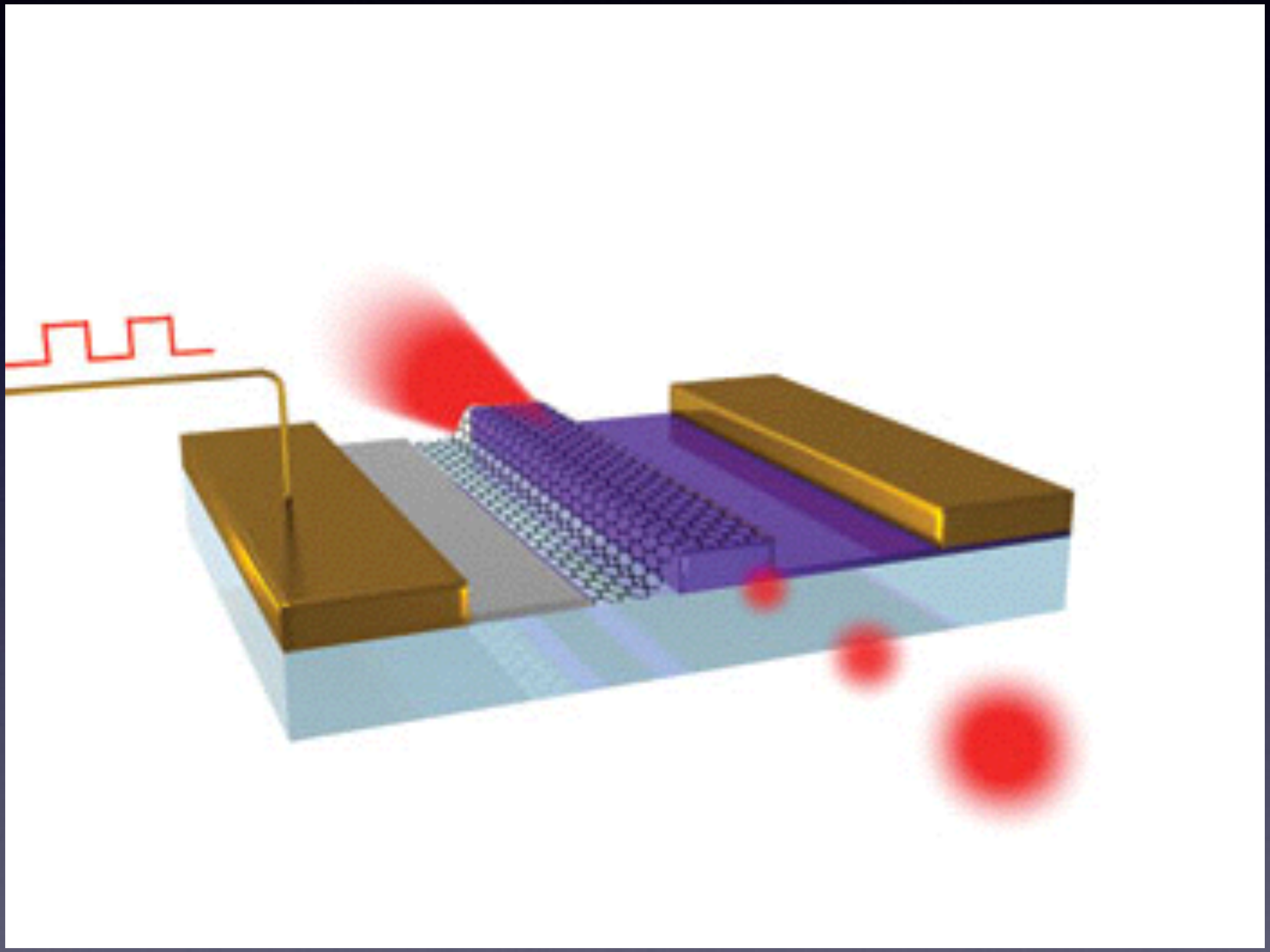
- In presence of a magnetic field, graphene layers can attract or repel each other, depending on the doping
- The force is quantised due to the quantised Hall effect
- Casimir force can be canceled by balancing doping and magnetic field. Important for quantum gravity!



Graphene optical modulators

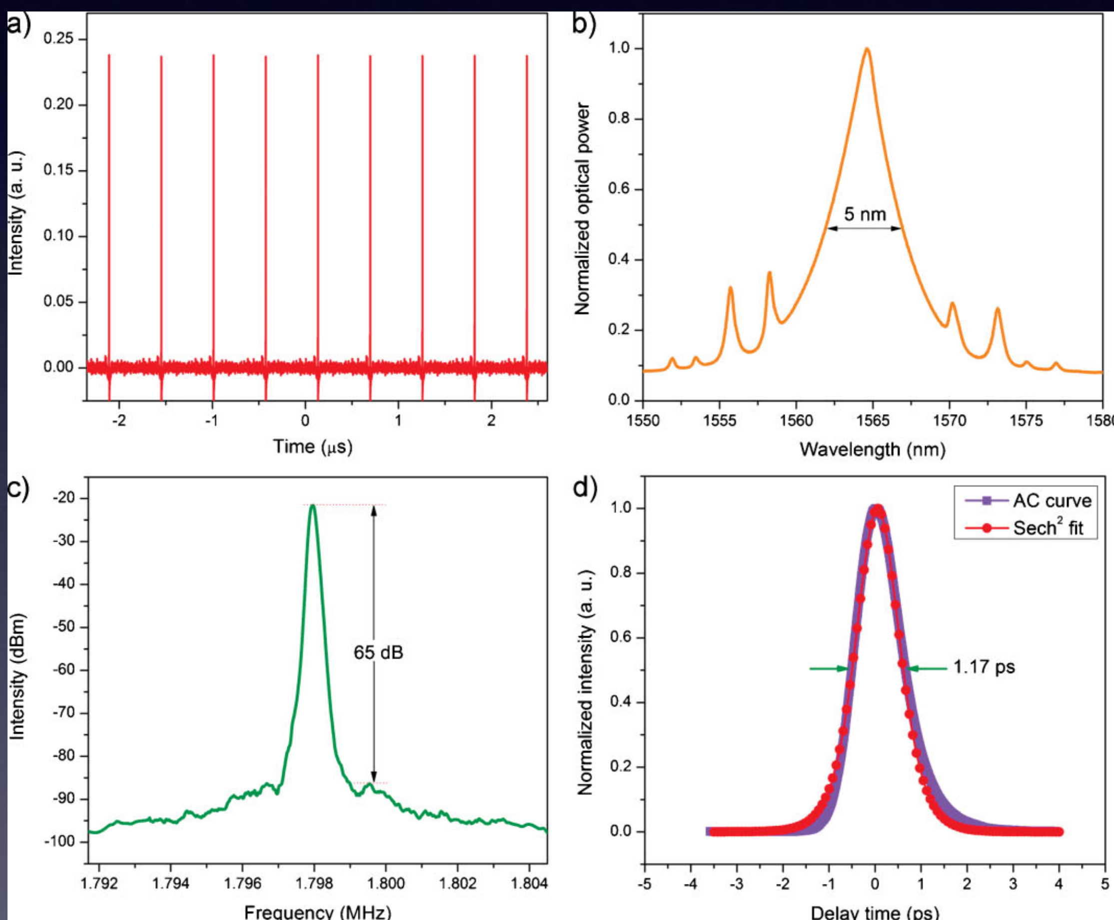
- Adjusting the Fermi energy to modulate light electrically

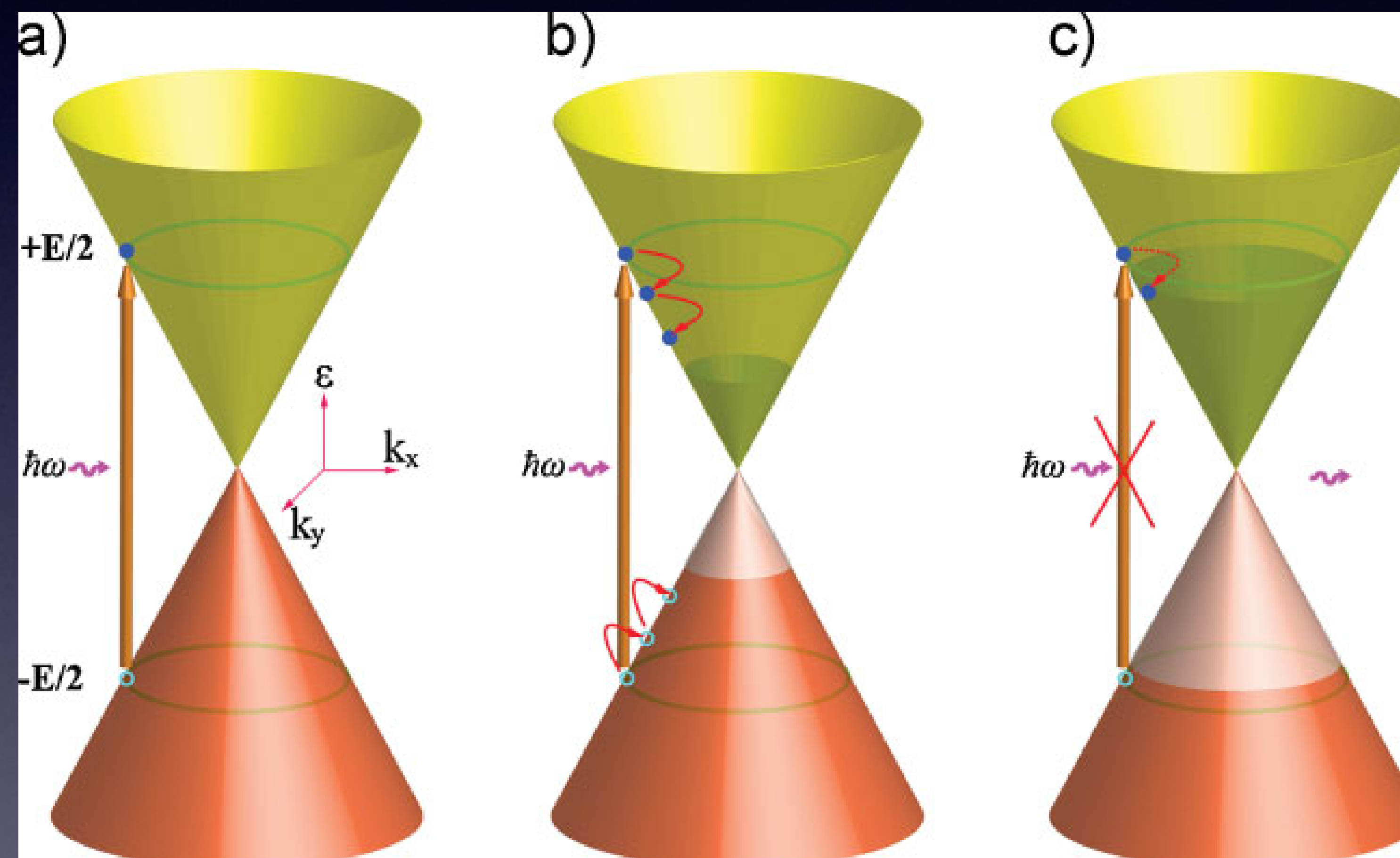




Saturable absorption

- Used in cavities to create trains of very short pulses





Atomic-Layer Graphene as a Saturable Absorber for Ultrafast Pulsed Lasers

By *Qiaoliang Bao, Han Zhang, Yu Wang, Zhenhua Ni, Yongli Yan, Ze Xiang Shen, Kian Ping Loh,** and *Ding Yuan Tang**

Graphene nonlinearity

- Conical dispersion of graphene gives a strong optical nonlinearity !

Mikhailov, 2009-2015

Linear energy dispersion ⇒ nonlinear electromagnetic response:

$$\dot{p}_x = -eE\cos\omega t, \quad p_x(t) \sim -(eE/\omega)\sin\omega t$$

$$v_x = v_F \frac{p_x}{p} \sim v_F \mathrm{sgn}(\sin\omega t)$$

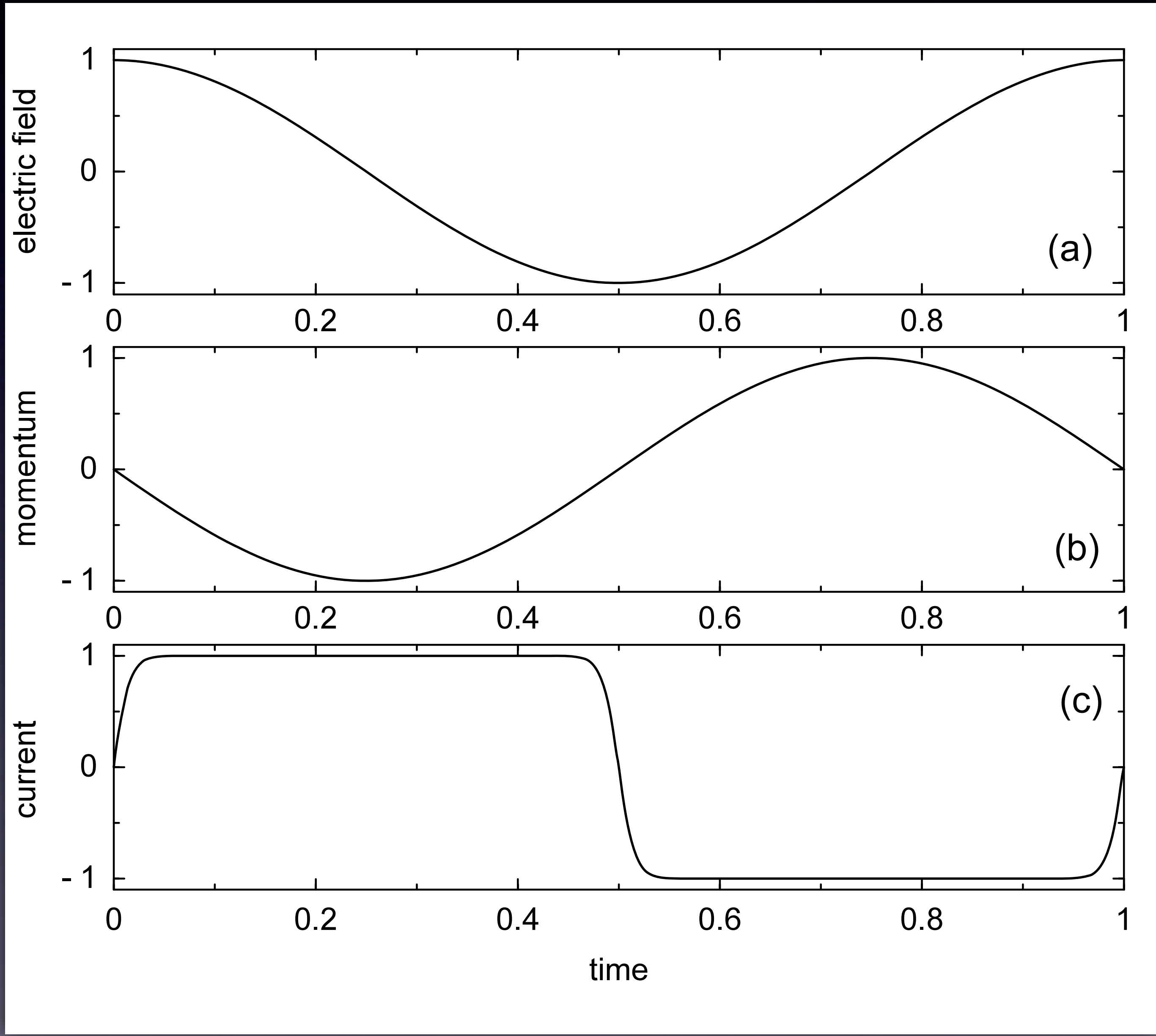
$$\sim v_F \frac{4}{\pi}\left\{\sin\omega t + \frac{1}{3}\sin 3\omega t + \frac{1}{5}\sin 5\omega t + \dots\right\}$$

Higher harmonics generation $\omega \Rightarrow m\omega$

Nonlinearity in graphene should be seen at much lower electric fields than in many other materials

Graphene current

- Graphene current is strongly nonlinear
- Sinusoidal excitation



$$\frac{\partial f_{\mathbf{p}}(\mathbf{r},t)}{\partial t} + \mathbf{v}_{\mathbf{p}}\frac{\partial f_{\mathbf{p}}(\mathbf{r},t)}{\partial \mathbf{r}} + \mathbf{F}(\mathbf{r},t)\frac{\partial f_{\mathbf{p}}(\mathbf{r},t)}{\partial \mathbf{p}} = 0$$

Doping controls the nonlinearity

Typical nonlinear electric field?

$$v_x = v_F \frac{p_x}{\sqrt{p_x^2 + p_y^2}}, \qquad -p_F \lesssim p_y \lesssim p_F, \qquad p_F = \hbar\sqrt{\pi n_s}$$

$$\Rightarrow \frac{v_x}{v_F} = \frac{p_x(t)}{|p_y|}\left(1 - \frac{p_x^2(t)}{2|p_y^2|}\right) \sim \frac{p_x(t)}{p_F}\left(1 - \frac{p_x^2(t)}{2|p_F^2|}\right)$$

Dimensionless electric field parameter in graphene

$$\mathcal{E}_{gr} \simeq \frac{eE}{p_F|\omega + i\gamma|}$$

if $\omega \gtrsim \gamma$, $f \simeq 1$ THz and $n_s \simeq 10^{11}$ cm^{-2}, then $\mathcal{E}_{gr} \simeq 1$ if

$$E \simeq 2 \times 10^3 \ \mathrm{V/cm}$$

Mikhailov, 2009-2015

Comparison with plasma nonlinearity

- Graphene:

$$\mathcal{E}_{gr} \simeq \frac{eE}{p_F|\omega + i\gamma|} \qquad E_{typical} \simeq 2 \times 10^3 \text{ V/cm}$$

- Conventional 3D plasma:

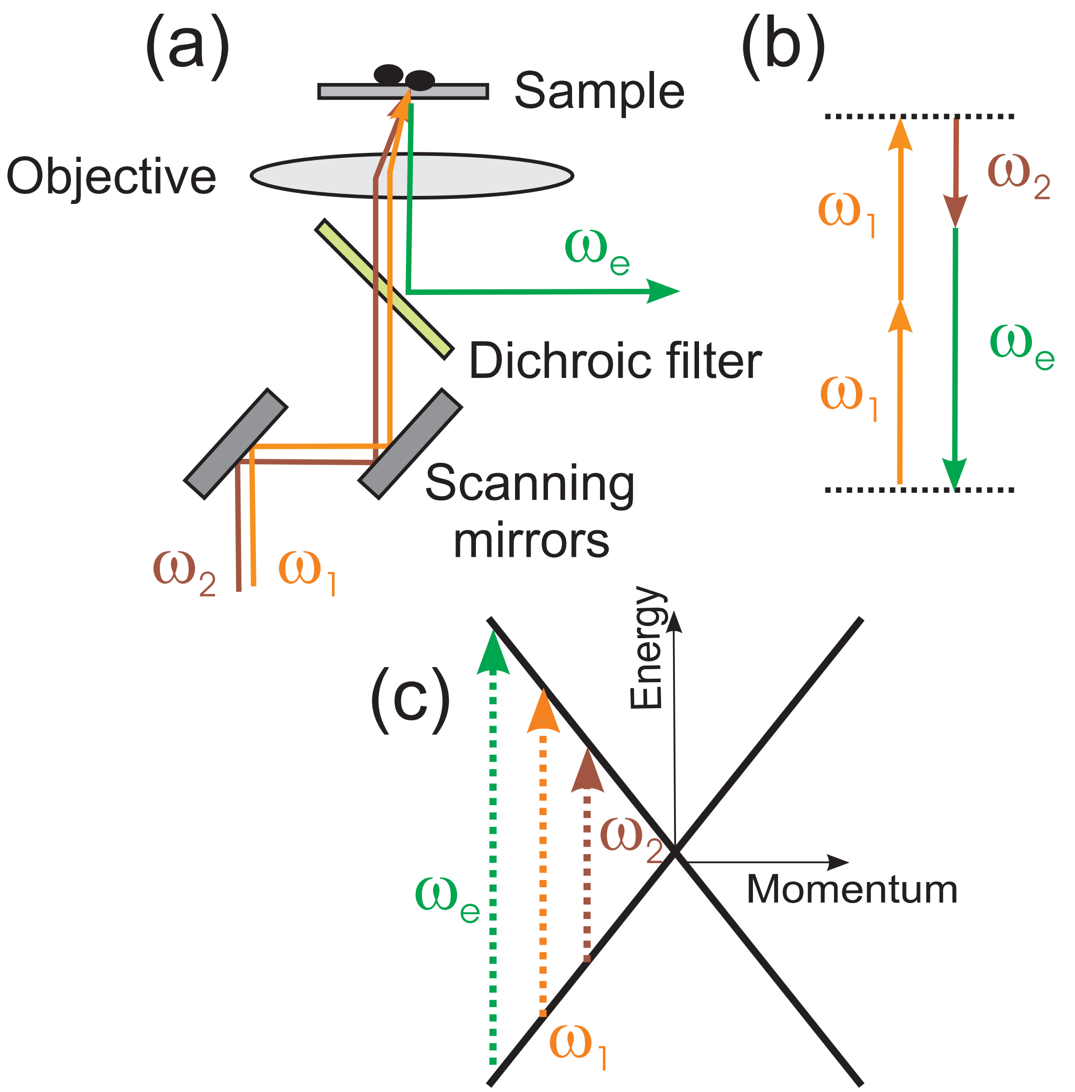
$$\mathcal{E}_{par} \simeq \frac{eE}{mc|\omega + i\gamma|} \qquad E_{typical} \simeq 10^8 \text{ V/cm}$$

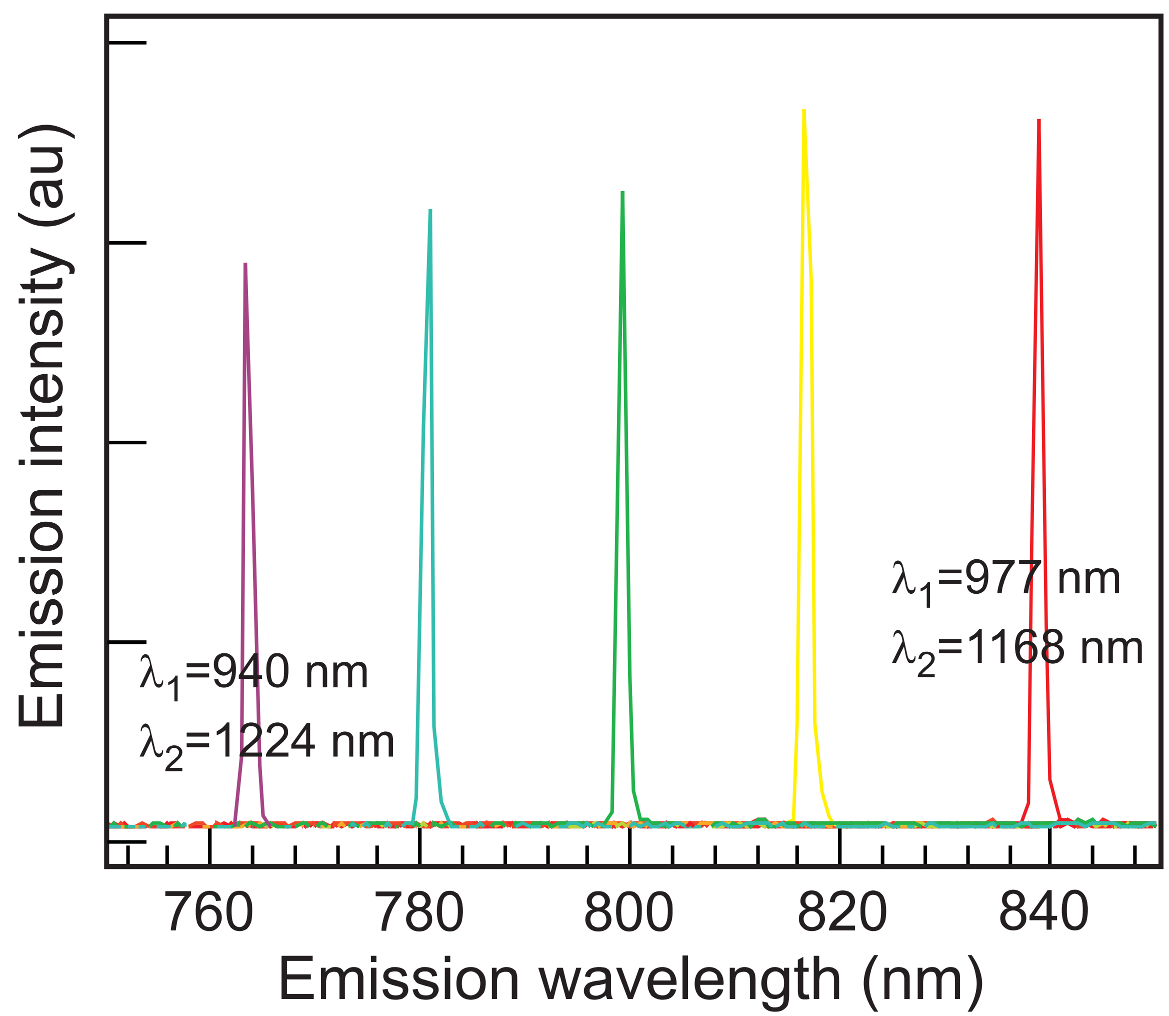
- Five orders of magnitude difference!
- 2nd and 3rd order effects $\propto \mathcal{E}^2$ and $\mathcal{E}^3 \Rightarrow$

Ten – fifteen orders of magnitude difference!

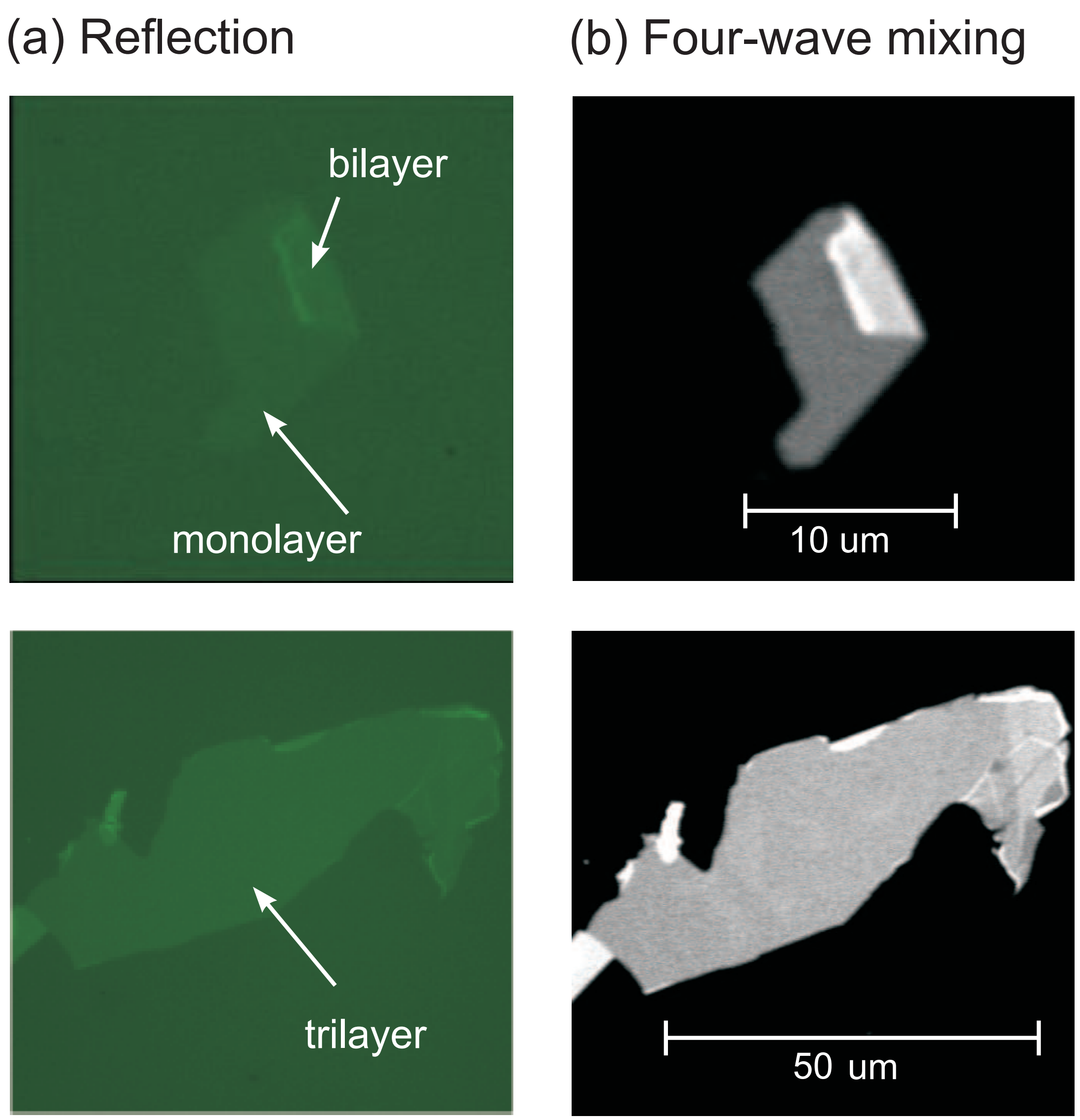
Four-wave mixing in graphene

Hendry et al, PRL'10





Four-wave mixing in graphene



Nonlinear susceptibility $\chi^{(3)}_{graphene}$:

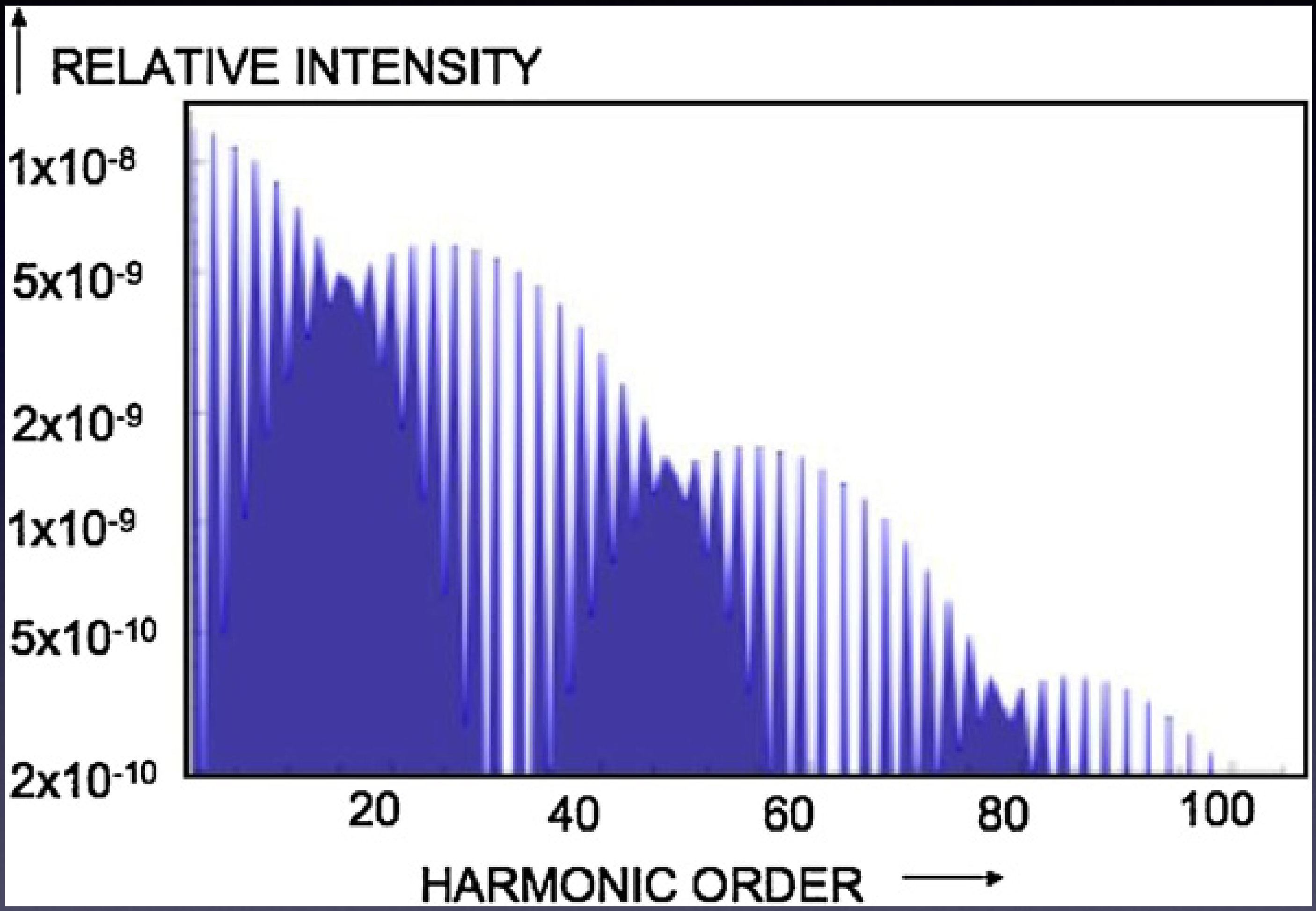
$$\chi^{(3)}_{gr} \simeq 10^{-7}\ \mathrm{esu}$$

- eight orders larger than in insulators
- $\sim$ 10 times larger than in gold
- about four orders larger than in InSb

Hendry, Mikhailov 2010

High-harmonic generation

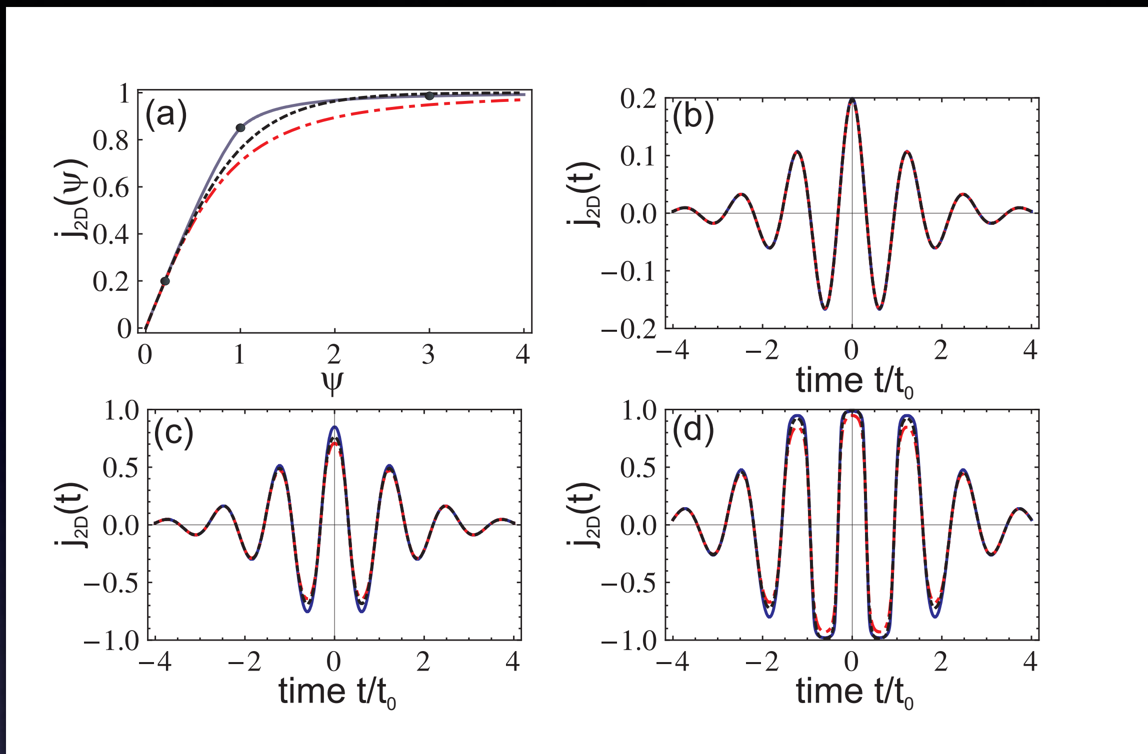
- THz pulse excitation
- Many high harmonics are observed in simulations
- Currently no experiments in the THz regime

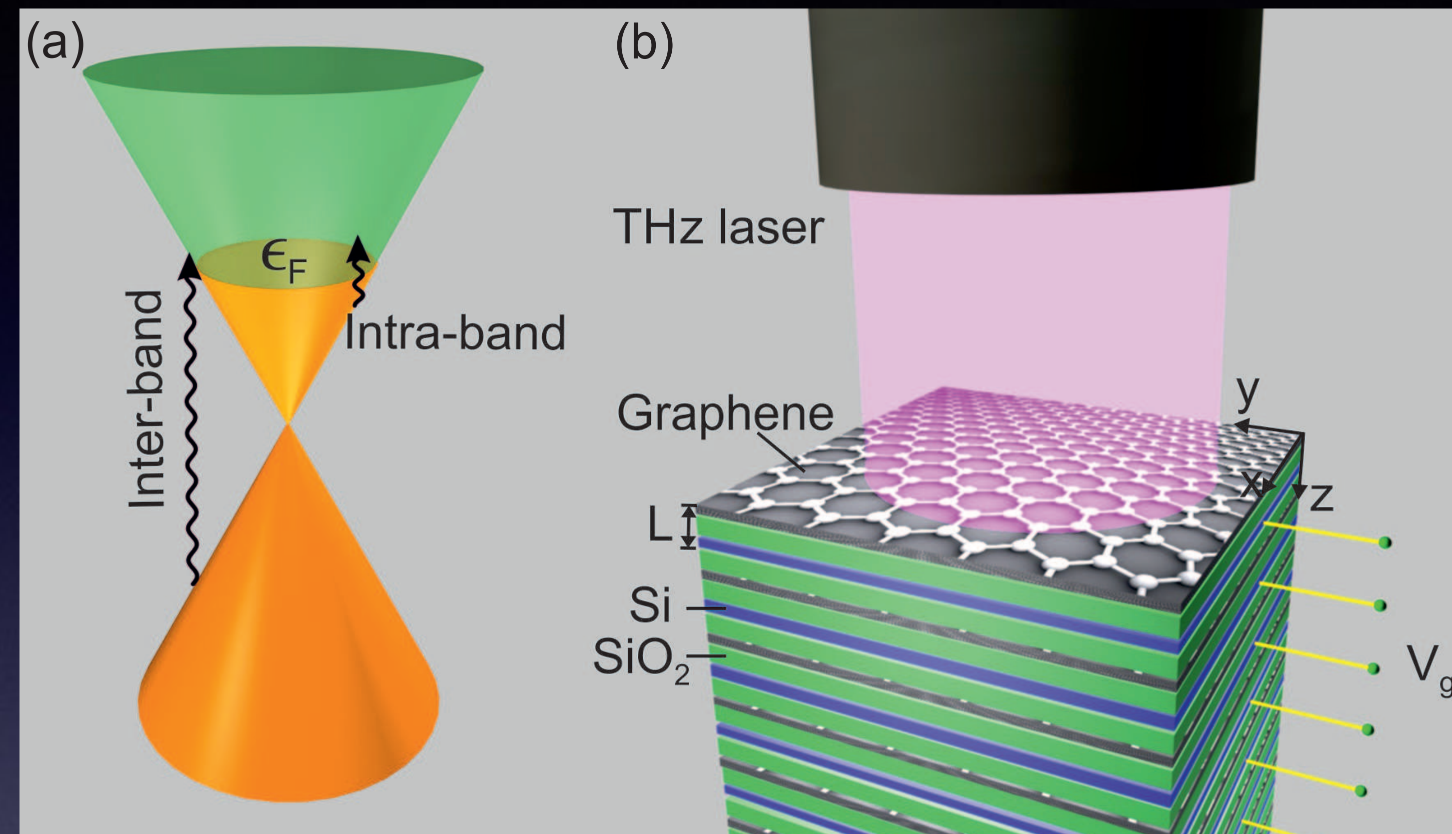


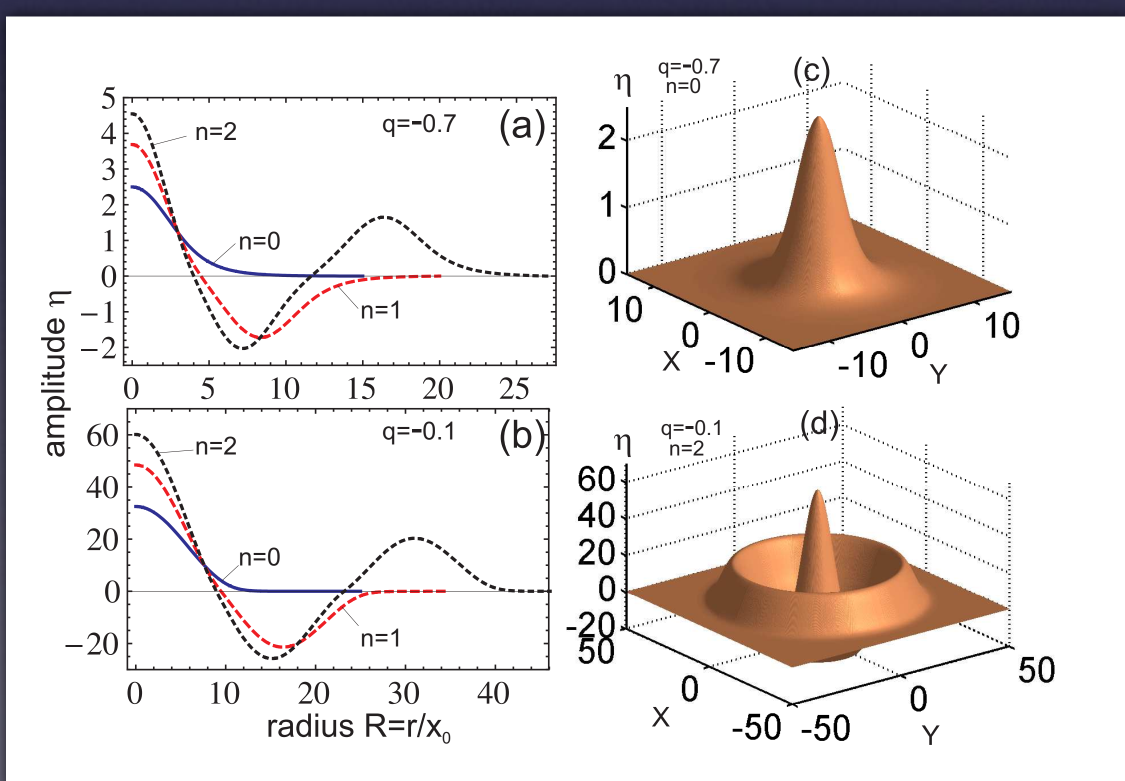
$$\chi^{(3)}_{\rm gr} = e^4 v_{\rm F}^2/(8\pi\epsilon_0\hbar^2\omega^4\epsilon_{\rm F} d) \sim 10^8 \div 10^{14}\chi^{(3)}_{\rm silica}$$

Biancalana-Conti, J. Phys. B 2013
Ishikawa 2012

Graphene metamaterials







$$i\hbar\partial_t\psi_p = v_{\rm F}\begin{bmatrix} 0 & (p_x + \frac{e}{c}A) - ip_y \\ (p_x + \frac{e}{c}A) + ip_y & 0 \end{bmatrix}\psi_p$$

$$J_{\rm 2D}(A) = -\frac{eg_{\rm s}g_{\rm v}v_{\rm F}}{(2\pi\hbar)^2}\frac{2|p_{\rm F}+eA|}{3eA}\left\{(p_{\rm F}^2+e^2A^2)\mathcal{E}_+\left(\frac{4eAp_{\rm F}}{(p_{\rm F}+eA)^2}\right) - (p_{\rm F}-eA)^2\mathcal{E}_-\left(\frac{4eAp_{\rm F}}{(p_{\rm F}+eA)^2}\right)\right\}$$

$$\left\{\left(\frac{\epsilon_{\rm s}\omega^2}{c^2} - k_0^2\right) + (\partial_x^2+\partial_y^2) + 2ik_0\partial_z\right\}\phi + \left[\frac{-e^2\epsilon_{\rm F}}{\pi\epsilon_0\hbar^2c^2d}\right]j_{\rm 2D}(\phi)c_0 = 0$$

Biancalana-Conti, J. Phys. B 2013

Theoretical models

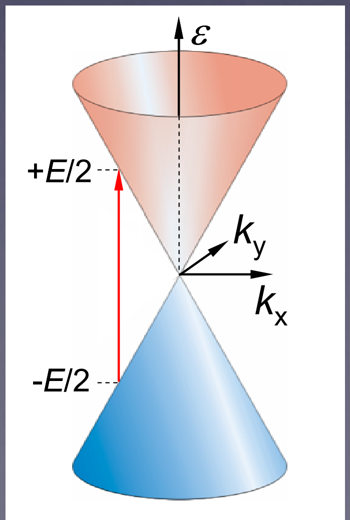
- Semiconductor Bloch equations adapted to the conical dispersion

Knorr, Malic, Koch

$$\dot{p}_k(t) = (i\Delta\omega_k + \Omega_k)\, p_k(t) - i\,\Omega_k^{\mathrm{vc}}\left[\rho_k^{\mathrm{c}}(t) - \rho_k^{\mathrm{v}}(t)\right] + \dot{p}_k(t)\Big|_{\mathrm{HF+s}}$$

$$\dot{\rho}_k^{\mathrm{v}}(t) = -2\,\mathrm{Im}\left[\Omega_k^{\mathrm{vc},*}\, p_k(t)\right] + \dot{\rho}_k^{\mathrm{v}}(t)\Big|_{\mathrm{HF+s}}\,,$$

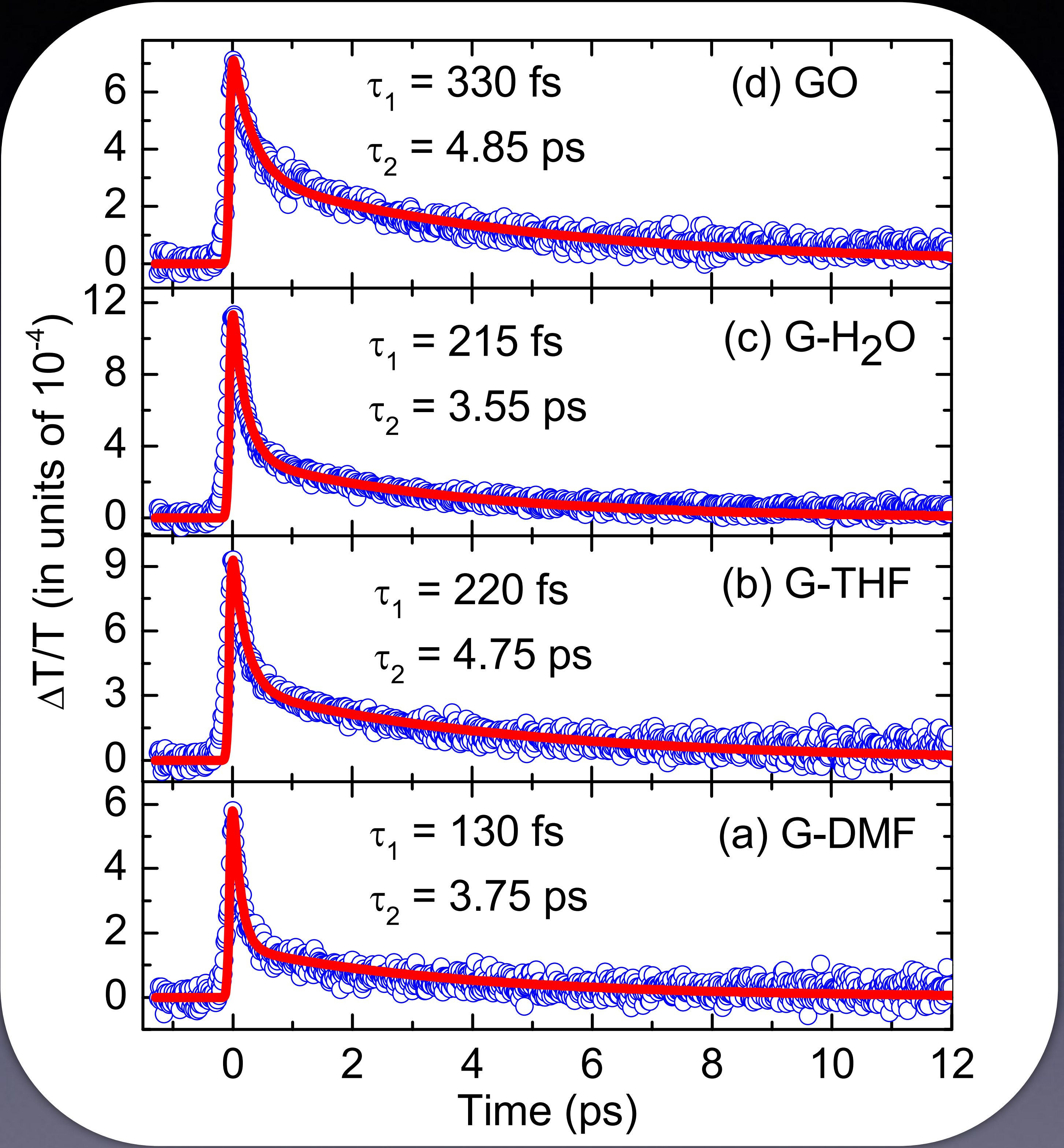
$$\dot{n}_q^j(t) = -\gamma_j\left[n_q^j(t) - n_{\mathrm{B}}\right] + \dot{n}_q^j(t)\Big|_{\mathrm{s}}\,.$$



- Collection of two-level systems, coupled by the **Coulomb interactions**
- Time-consuming but allegedly precise

Relaxation times

- Relaxation times vary enormously depending on the substrate or the suspension
- There is a strong electronic interaction with the substrate



Ishikawa's equations

Ishikawa 2012

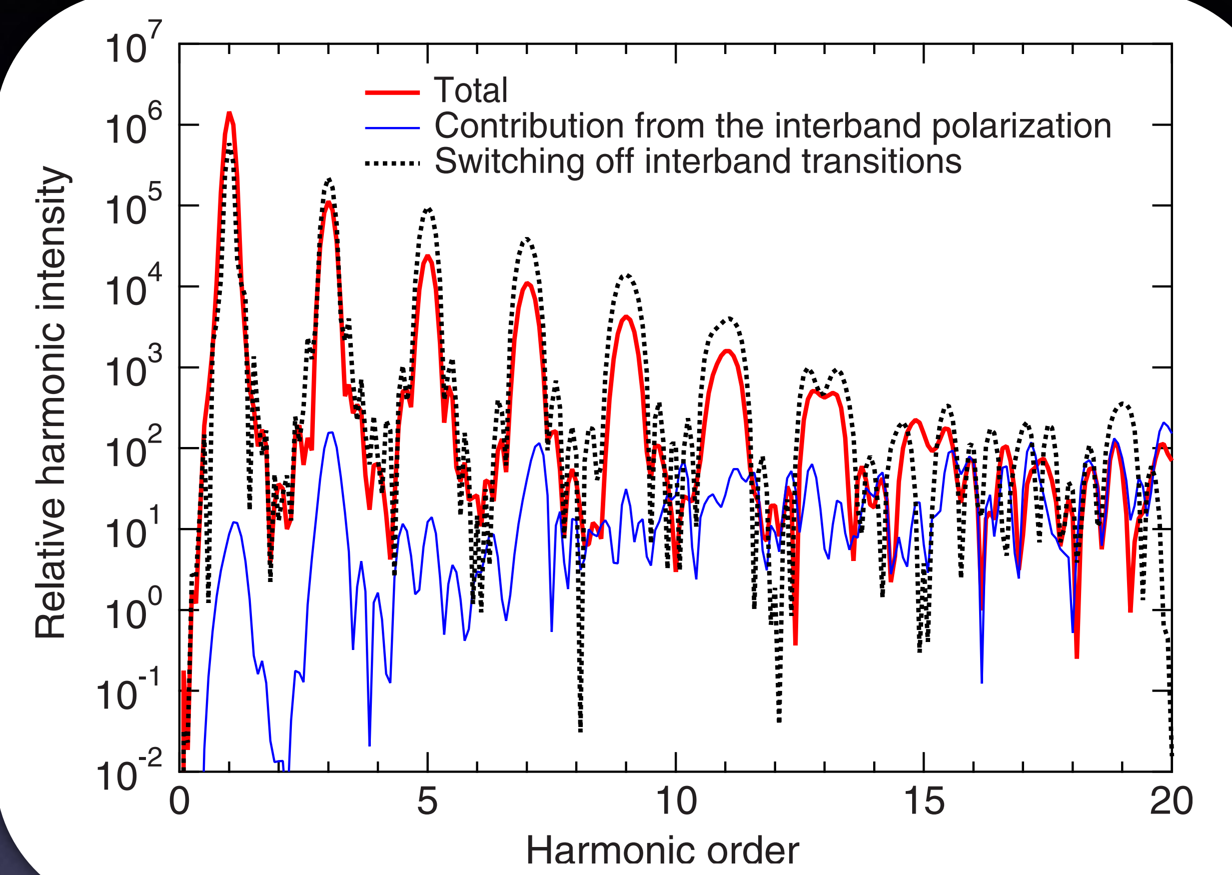
$$i\hbar\frac{\partial}{\partial t}\psi = v_F\begin{pmatrix}0 & pe^{-i\phi}+eA(t)\\ pe^{i\phi}+eA(t) & 0\end{pmatrix}\psi$$

$$\dot{\rho} = -\frac{\mathrm{i}}{2}\dot{\theta}(t)n(t)\,\mathrm{e}^{2\mathrm{i}\Omega(t)},$$

$$\dot{n} = -\mathrm{i}\,\dot{\theta}(t)\rho(t)\,\mathrm{e}^{-2\mathrm{i}\Omega(t)} + \mathrm{c.c.}$$

$$\Omega(t)=\frac{v_F}{\hbar}\int\sqrt{[p_x+eA(t)]^2+p_y^2}\,dt$$

$$\dot{\theta}(t) = \frac{p_y eE(t)}{[p_x+eA(t)]^2+p_y^2}$$



- No Coulomb interactions are accounted for

$$\mathbf{J}(t) = -\frac{g_s g_v e}{(2\pi\hbar)^2}\int \mathbf{j}_{\mathrm{c}}(t)\,d\mathbf{p}$$

Ishikawa's equations

Biancalana 2015

$$i\hbar\frac{\partial}{\partial t}\psi = v_F\begin{pmatrix} 0 & pe^{-i\phi} + eA(t) \\ pe^{i\phi} + eA(t) & 0 \end{pmatrix}\psi$$

$$\dot{\rho} = -\frac{\mathrm{i}}{2}\dot{\theta}(t)n(t)\,\mathrm{e}^{2\mathrm{i}\Omega(t)},$$

$$\dot{n} = -\mathrm{i}\,\dot{\theta}(t)\rho(t)\,\mathrm{e}^{-2\mathrm{i}\Omega(t)} + \mathrm{c.c.}$$

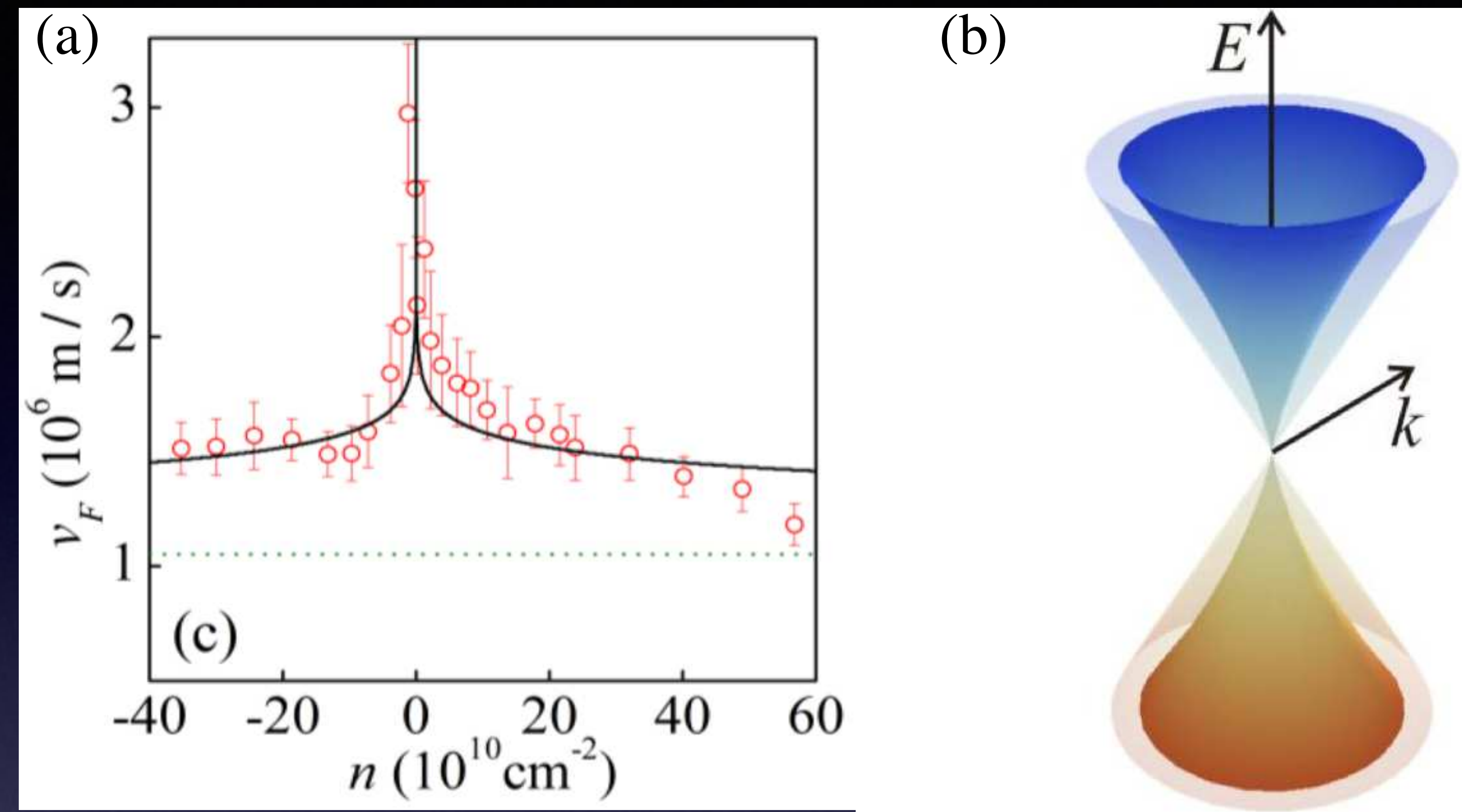
$$\Omega(t) = \frac{v_F}{\hbar}\int\sqrt{[p_x + eA(t)]^2 + p_y^2}\,dt$$

$$\dot{\theta}(t) = \frac{p_y eE(t)}{[p_x + eA(t)]^2 + p_y^2}$$

- SBEs are not adequate to describe short pulses interacting with graphene
- Even long pulses "feel" the Dirac point
- The differences are very often dramatic

Coulomb interactions in graphene ?!

- Coulomb interactions should spoil the law of universal absorption
- Several works predict the renormalisation of the Fermi velocity near the Dirac point, when doping is present
- Without doping, Coulomb interactions seem to be irrelevant!



$$\alpha = \frac{e^2}{\kappa v_F}$$

$$\alpha = 2.2$$

PRL **113,** 105502 (2014) PHYSICAL REVIEW LETTERS week ending 5 SEPTEMBER 2014

Why Does Graphene Behave as a Weakly Interacting System?

Johannes Hofmann,* Edwin Barnes, and S. Das Sarma
Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA
(Received 6 June 2014; published 5 September 2014)

Z-scan measurements (Heriot-Watt)

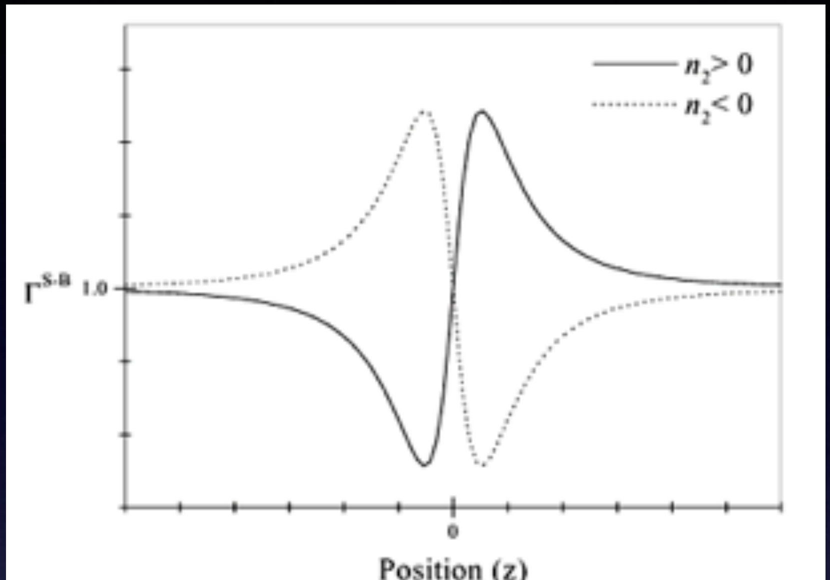
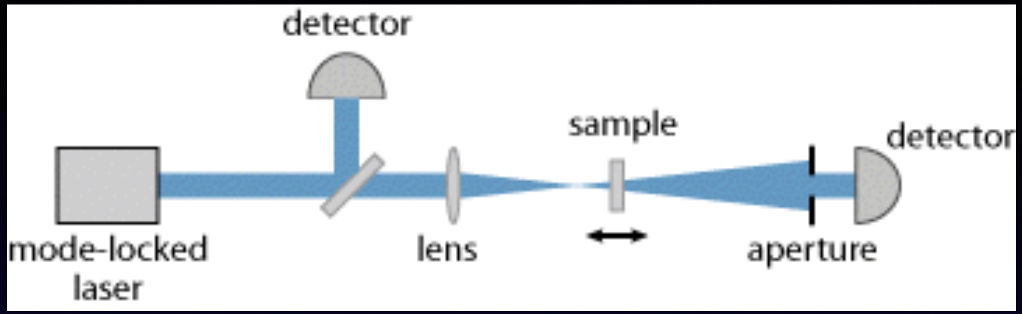
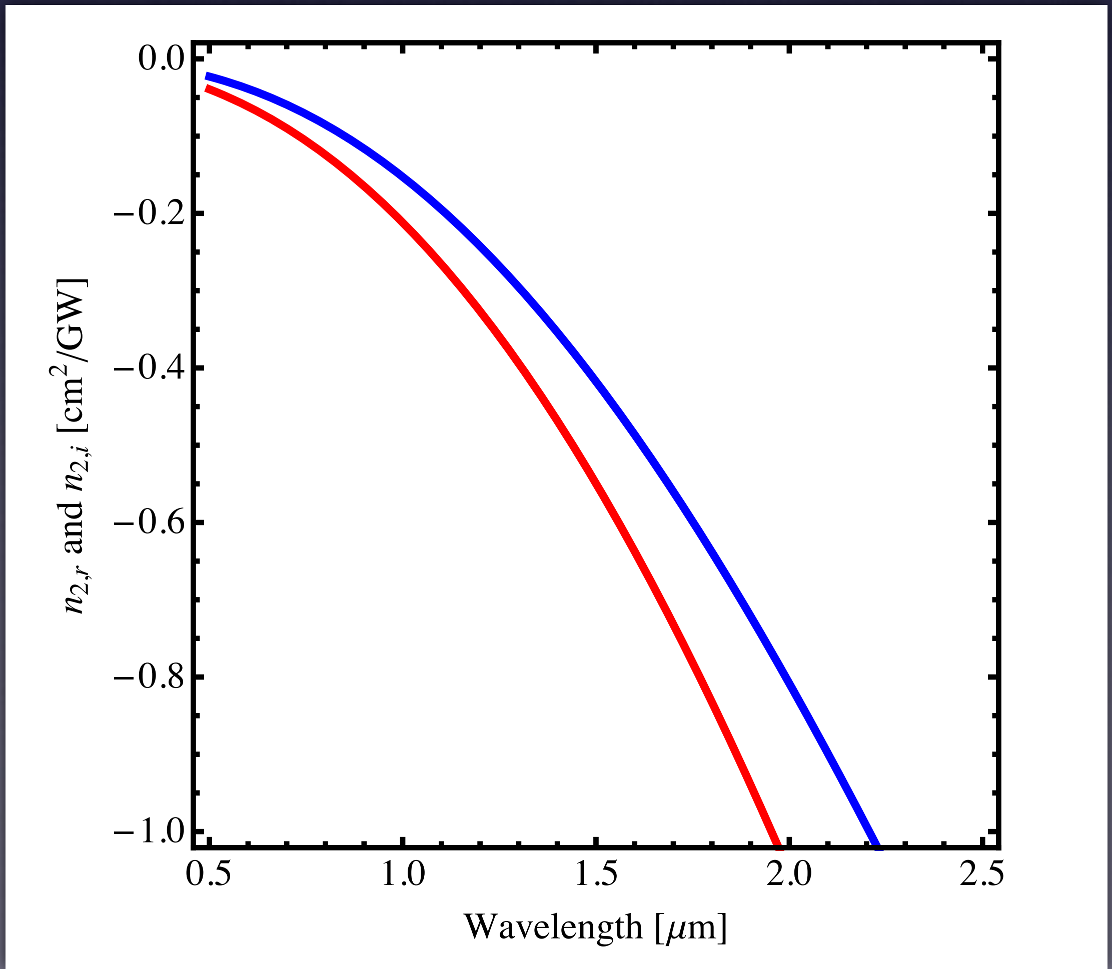
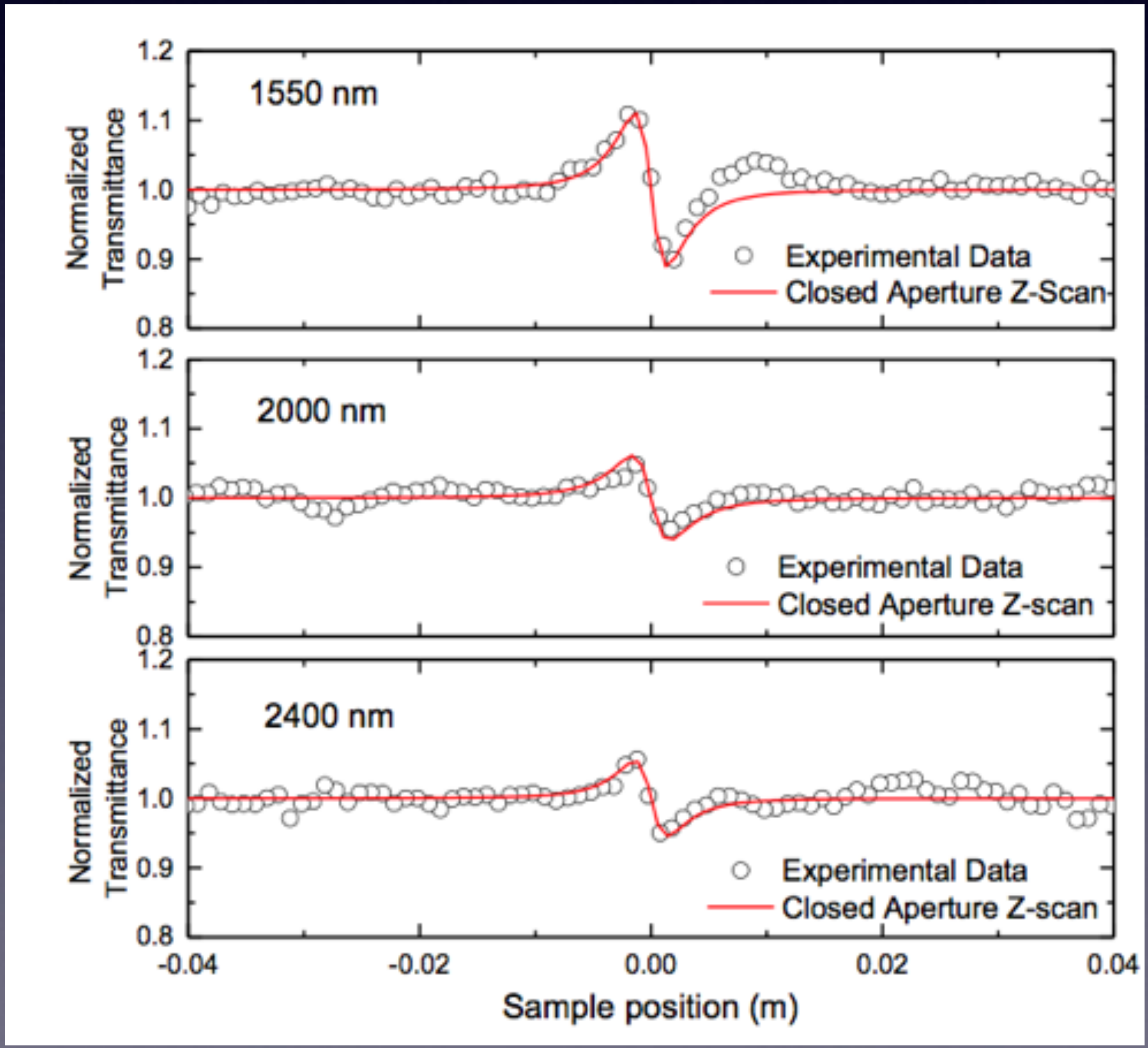


Figure 2. Z-scan theoretical curves of the transmittance as a function of z, obtained with Eq. 5.

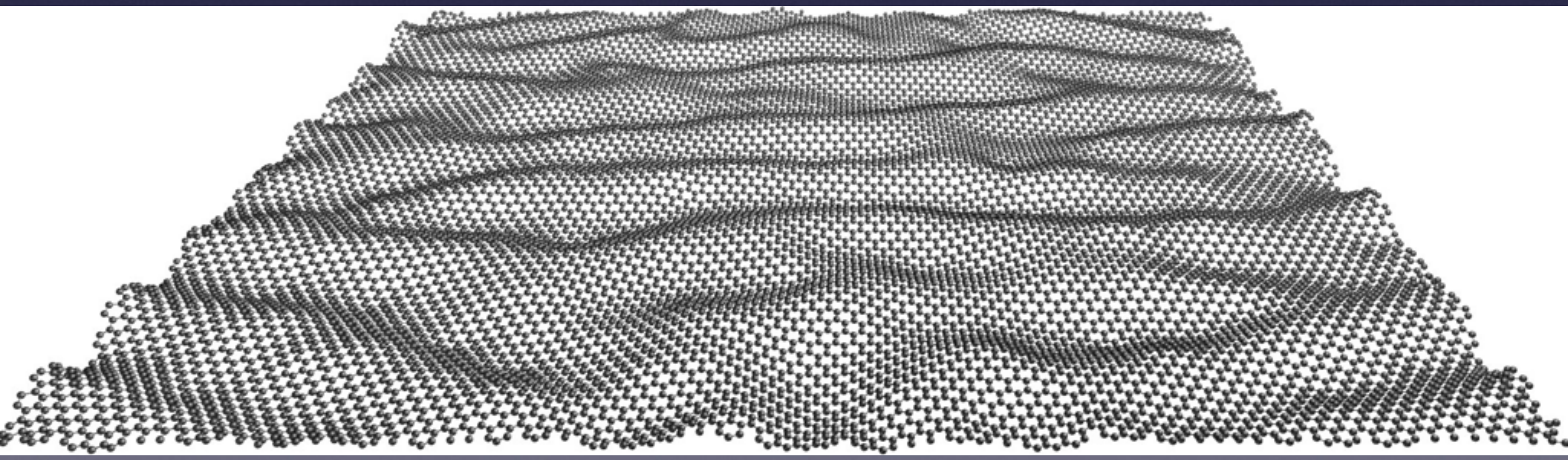






Sound waves in graphene

- Transverse and Flexural phonons = 3 branches like in 3D
- Described by General Relativity !!
- Can graphene phonons be described by 2D quantum gravity?



M. Vozmediano

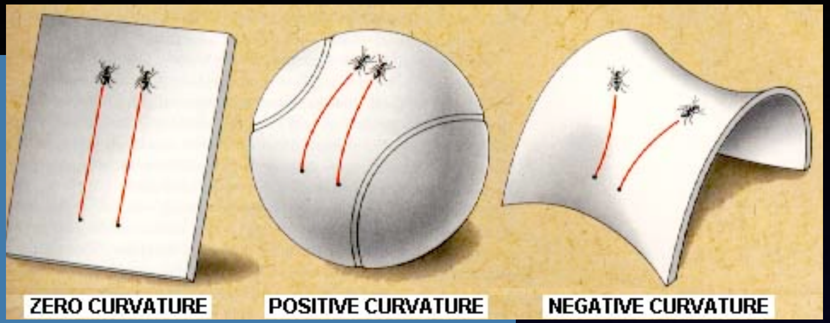
Curvature in graphene

Physical origin of the curvature

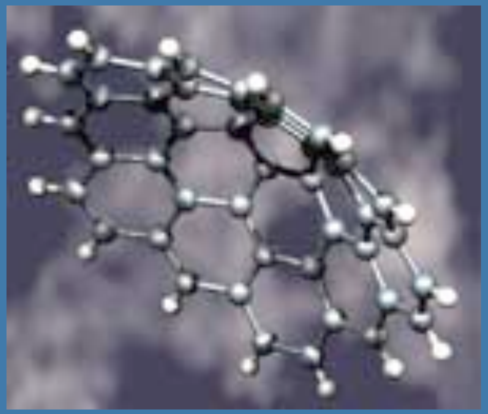
- Elastic fluctuations (very unlikely).
- Interaction with the substrate –observed, but ripples are also observed in suspended samples-.
- Topological defects. The only way to introduce curvature in 2D.

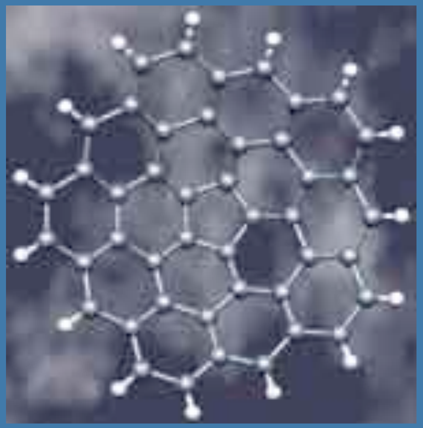
Present in previous graphene-like structures (nanotubes, fullerenes and bombarded graphite).

Topological defects

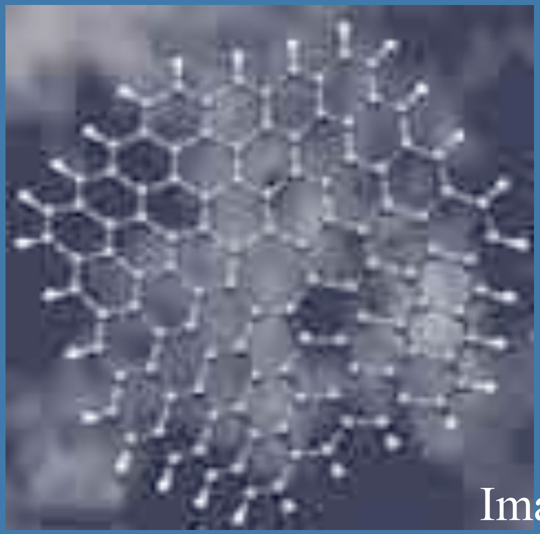


Topological defects



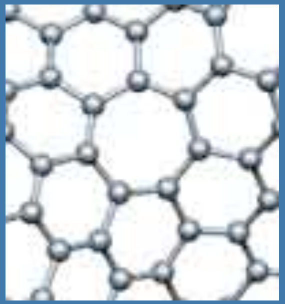


Topological defects are formed by replacing a hexagon by a n-sided polygon



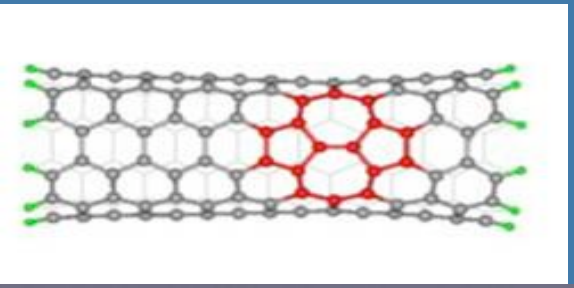
Images: C. Ewels

Pentagon: induces positive curvature



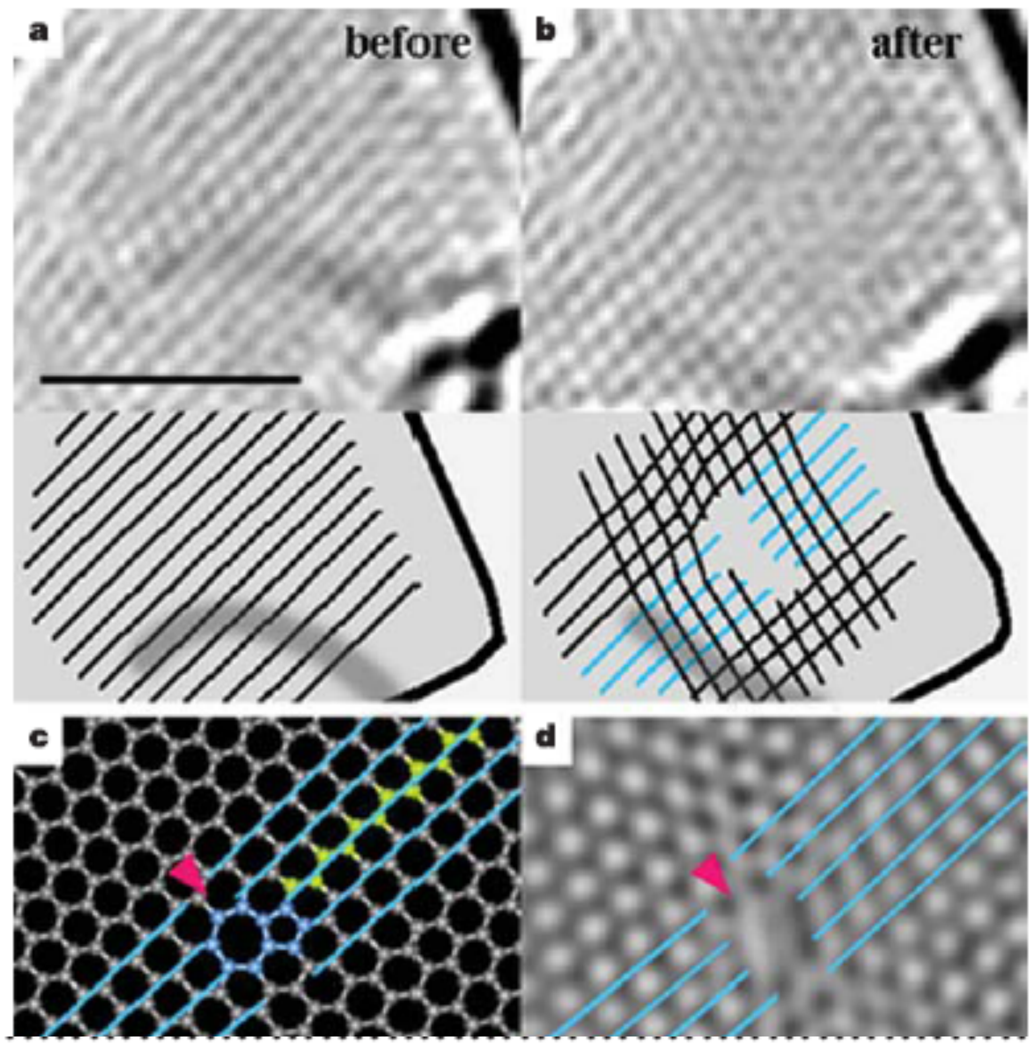
Heptagon: induces negative curvature

The combination of a pentagon and an heptagon at short distances can be seen as a dislocation of the lattice.



The most common defects in nanotubes are made by pentagons, heptagons, and pairs of them (Stone-Wales defects)

Observation of topological defects in graphene



Direct evidence for atomic defects in graphene layers

Ayako Hashimoto[1], Kazu Suenaga[1], Alexandre Gloter[1,2], Koki Urita[1,3] & Sumio Iijima[1]

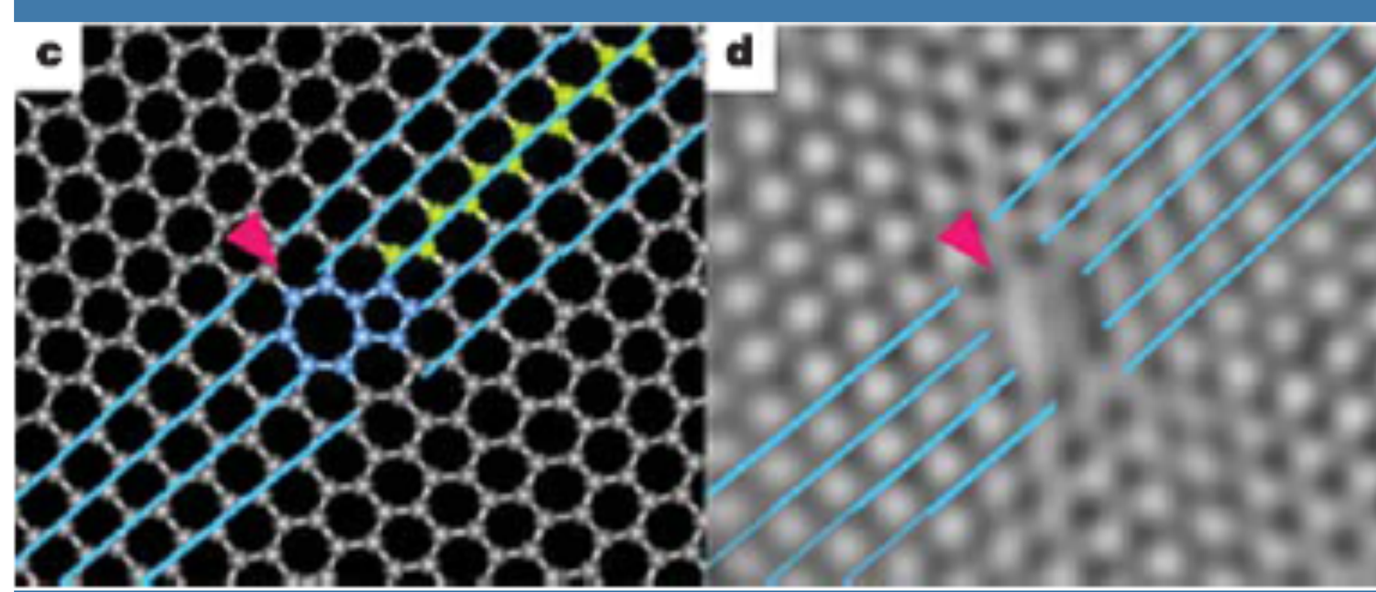
Nature 430 (2004)

model of the pentagon–heptagon pair in the graphitic network. **d**, A simulated HR-TEM image shows a good comparison with the HR-TEM image showin in **b**. Scale bar, 2 nm.

In situ of defect formation in single graphene layers by high-resolution TEM.

Defects must be present in all graphene samples and have a strong influence on the electronic properties

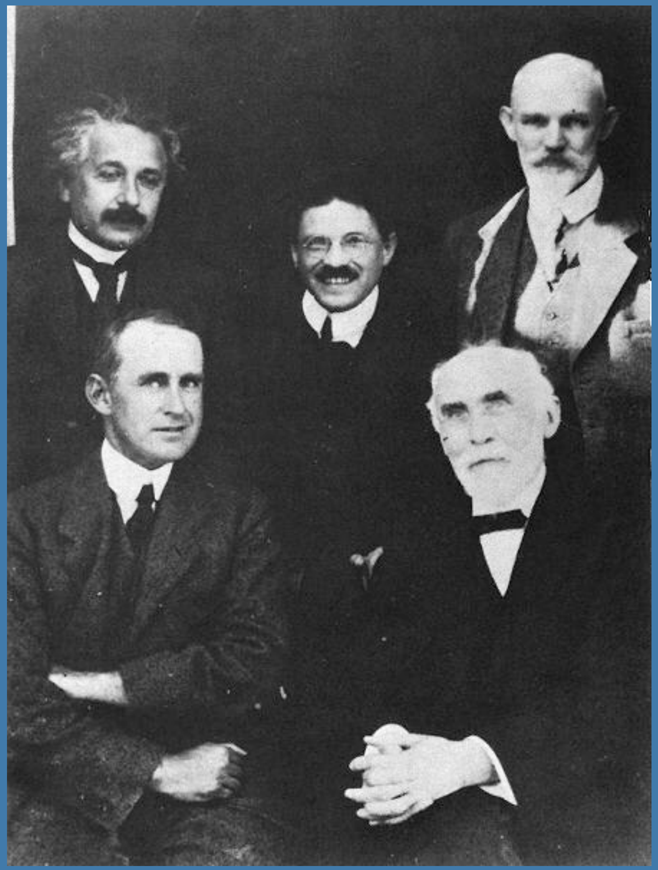
Vacancies
Ad-atoms
Edges
Topological defects



Fermions in curved space

Dirac in curved space

We can include curvature effects by coupling the Dirac equation to a curved space



$$\gamma^a e_a^\mu \left(\partial_\mu - \Omega_\mu(x)\right)\psi = E\Psi$$

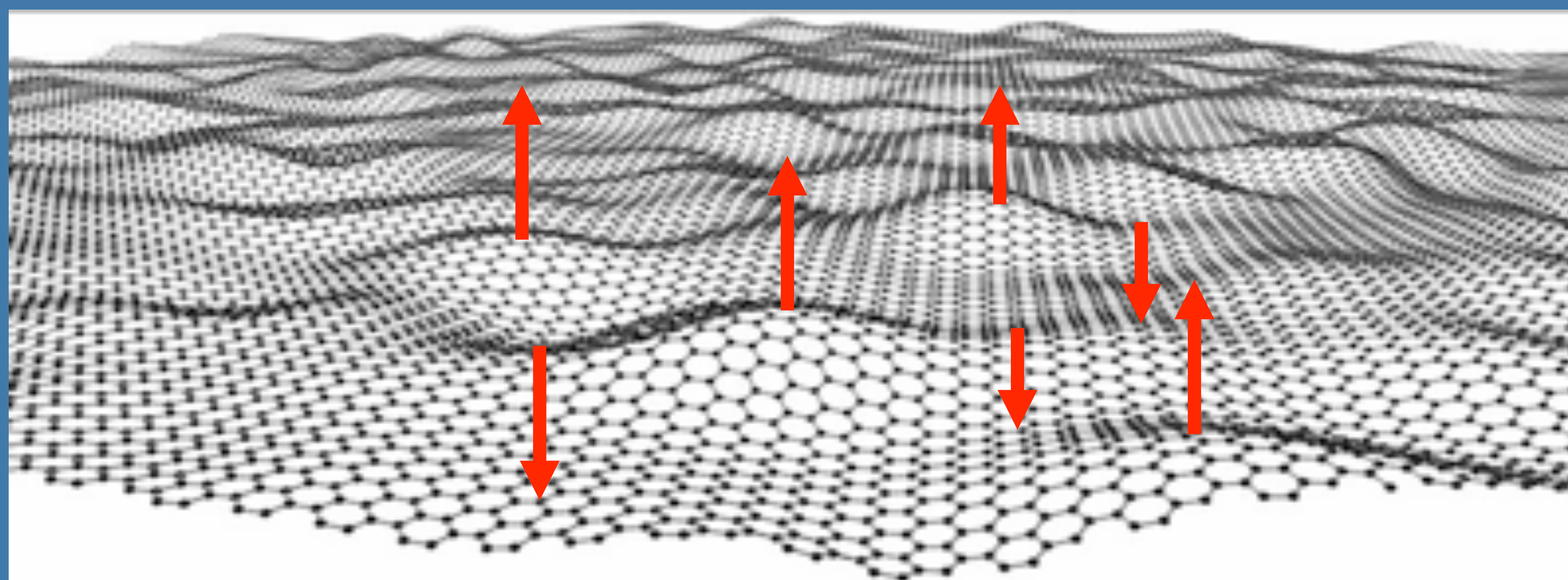
Need a metric and a "tetrad".

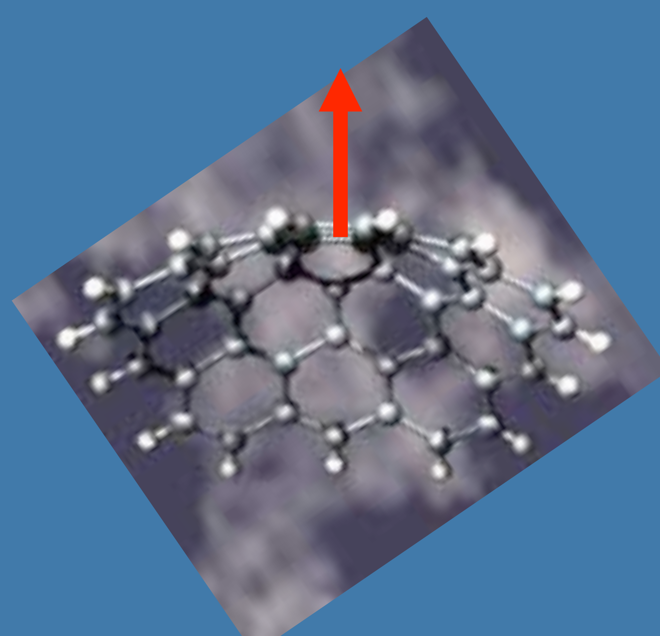
$$e_\mu^a e_\nu^b \eta_{ab} = g_{\mu\nu}$$

Generate r-dependent Dirac matrices and an effective "gauge" field.

$$\Omega_\mu = \frac{1}{4}\gamma^a\gamma^b e^\nu_{a;\mu} e_{b\nu}$$

Modeling ripples in flat samples with topological defetcs

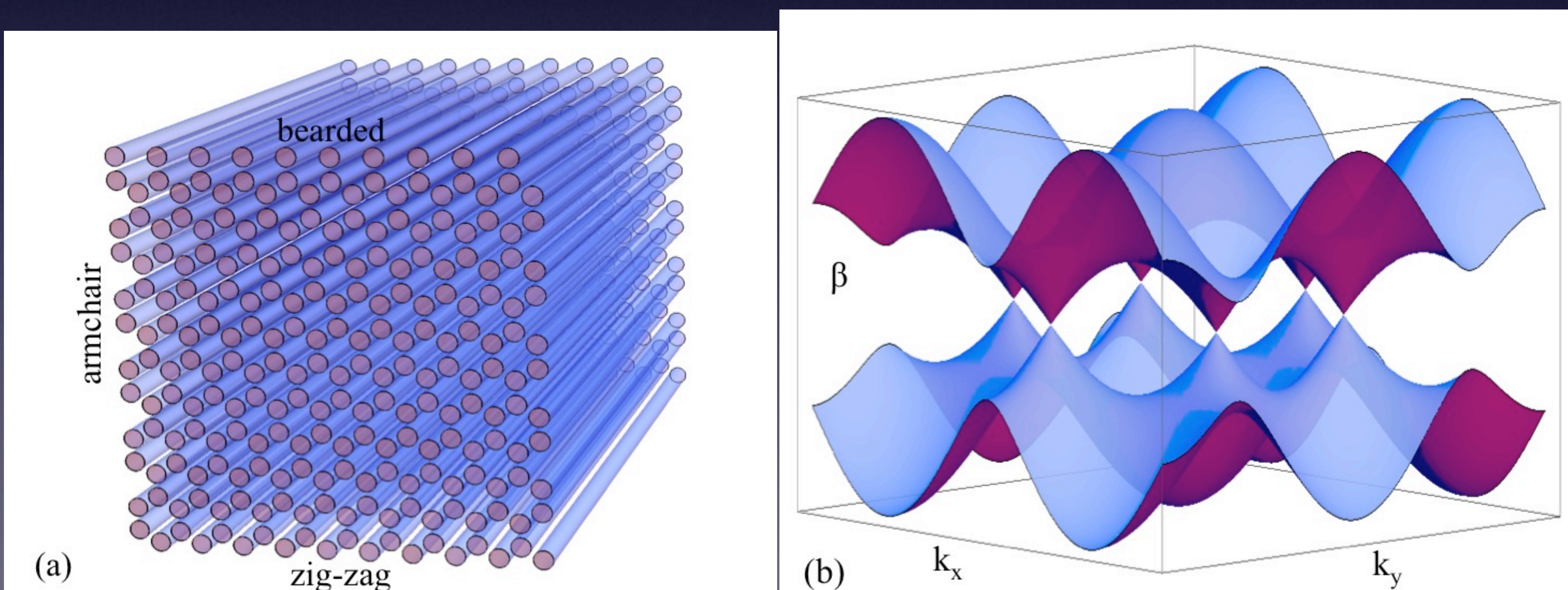




Use an equal number of 5 and 7 rings

Photonic graphene

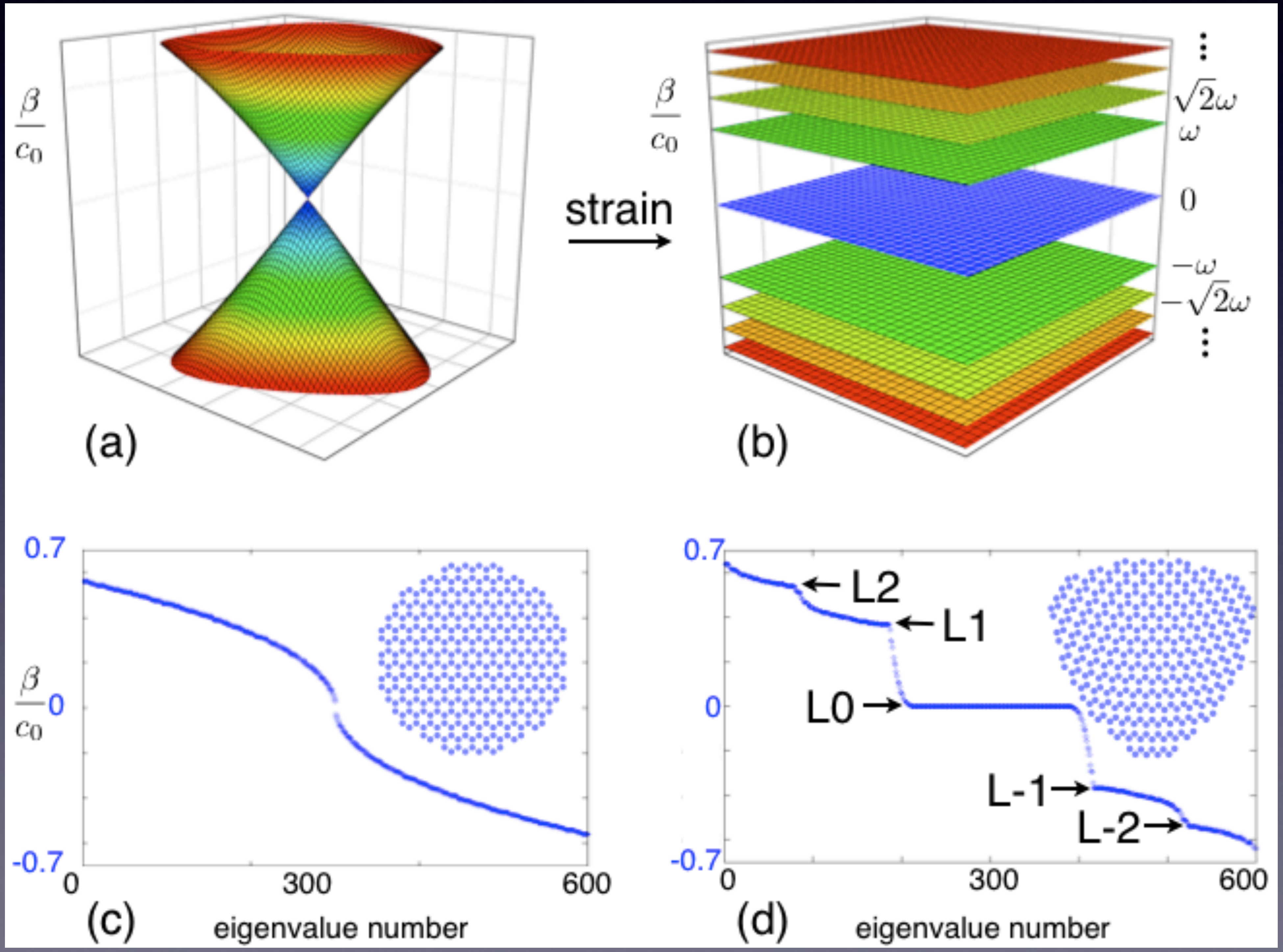
- Arrays of waveguides arranged with the honeycomb structure
- Mechanical strain can be applied



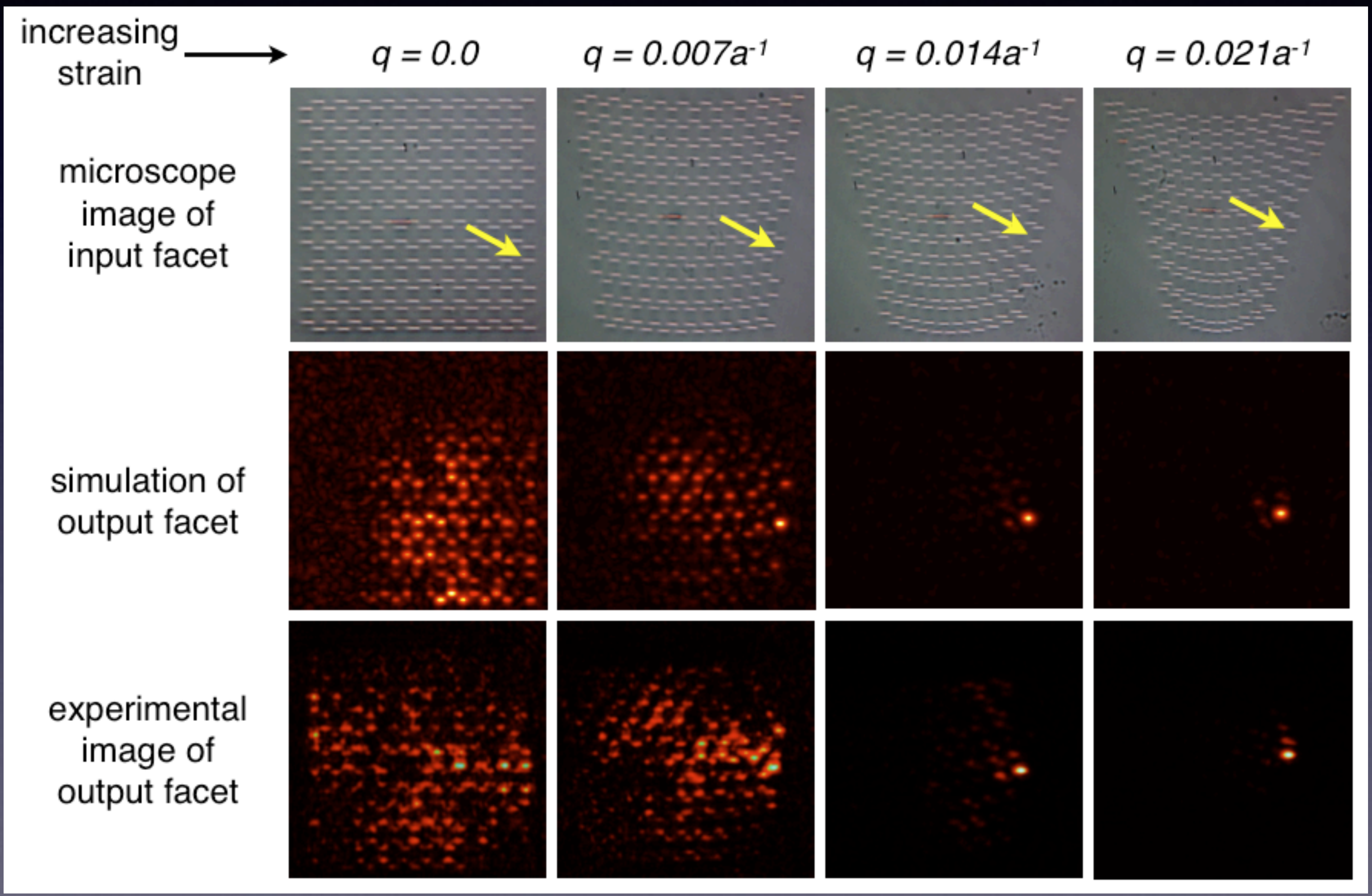
A. Szameit

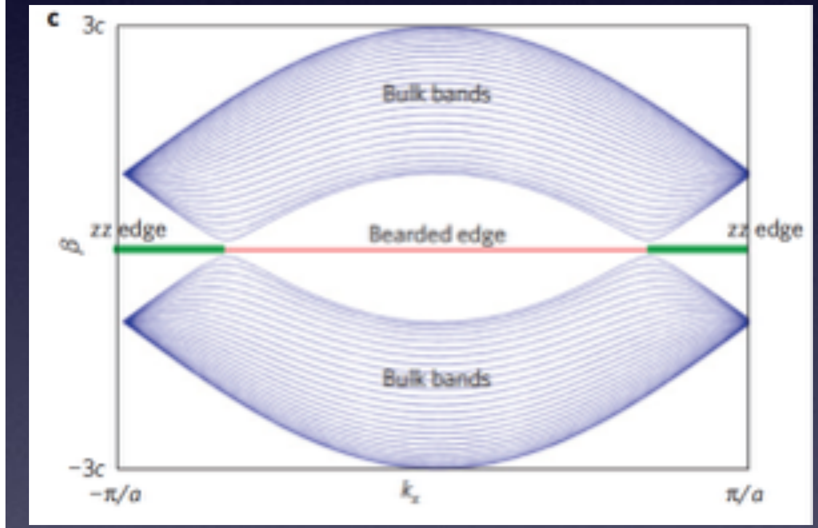
Artificial magnetic fields

- Strain-induced artificial gauge fields - and Landau levels



Edge states





A. Szameit

Conclusions

- Graphene has potentially important practical applications
- Test-bed for QFT, particle physics, gravity, biophysics and who knows what else
- Interesting nonlinear optical properties, solitons, high-harmonic generation and four-wave mixing