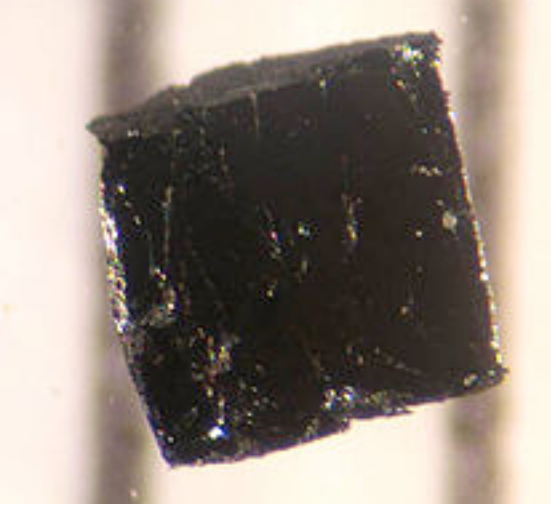
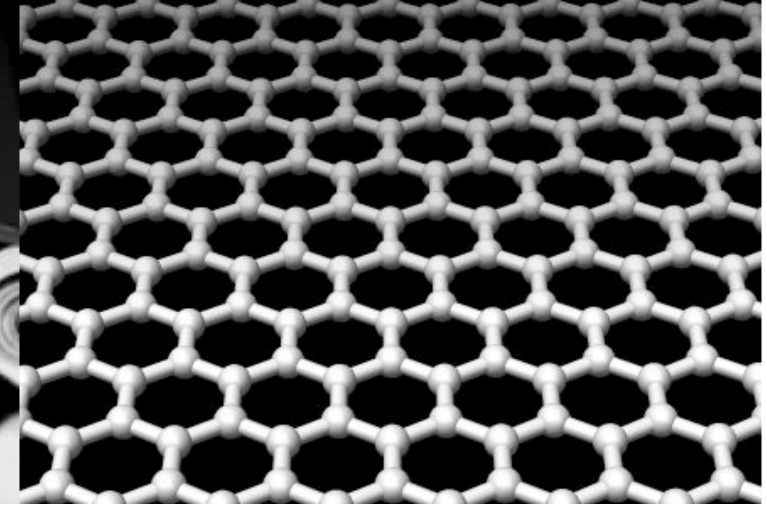
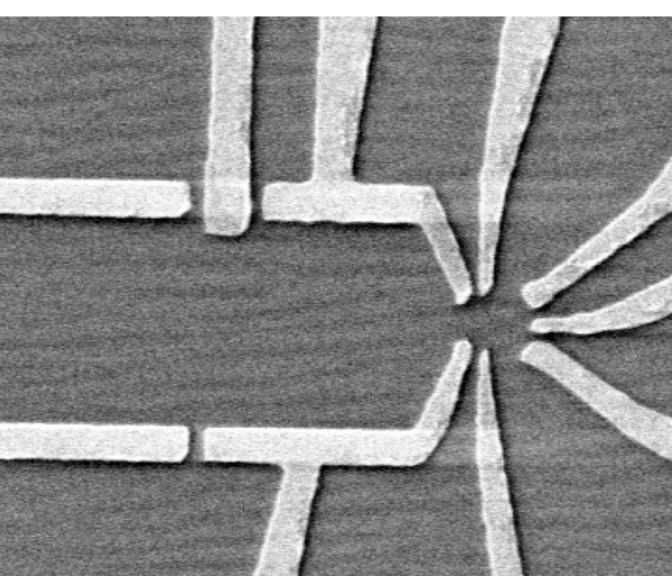




# Modeling in Physics

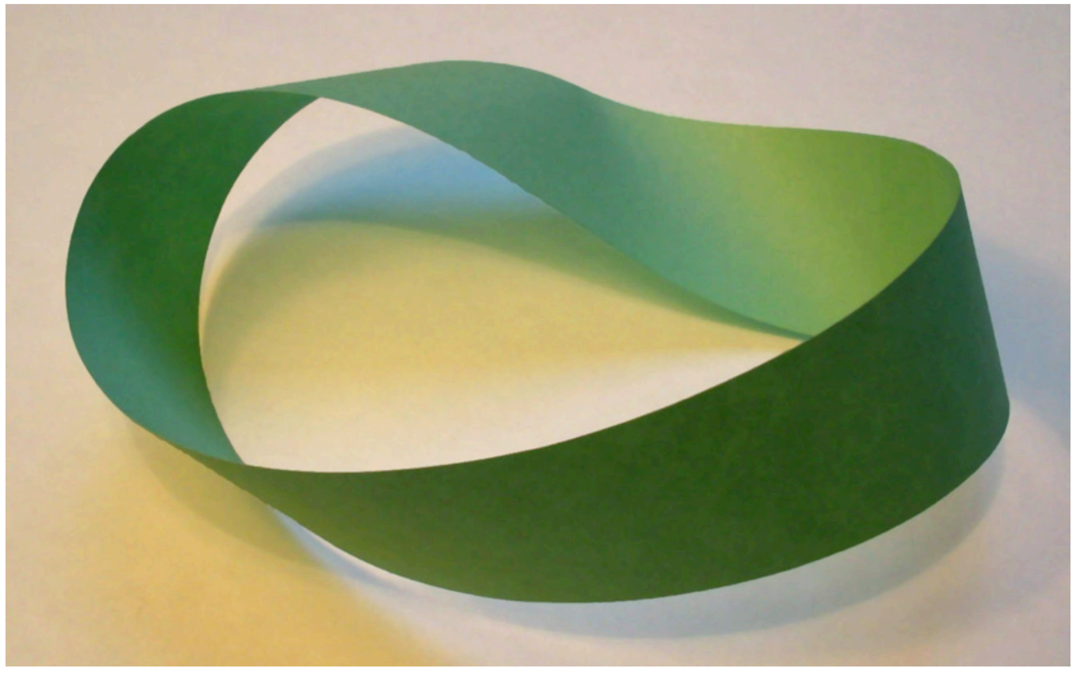

Bruno Uchoa
Department of Physics and Astronomy
University of Oklahoma


# Lecture 4

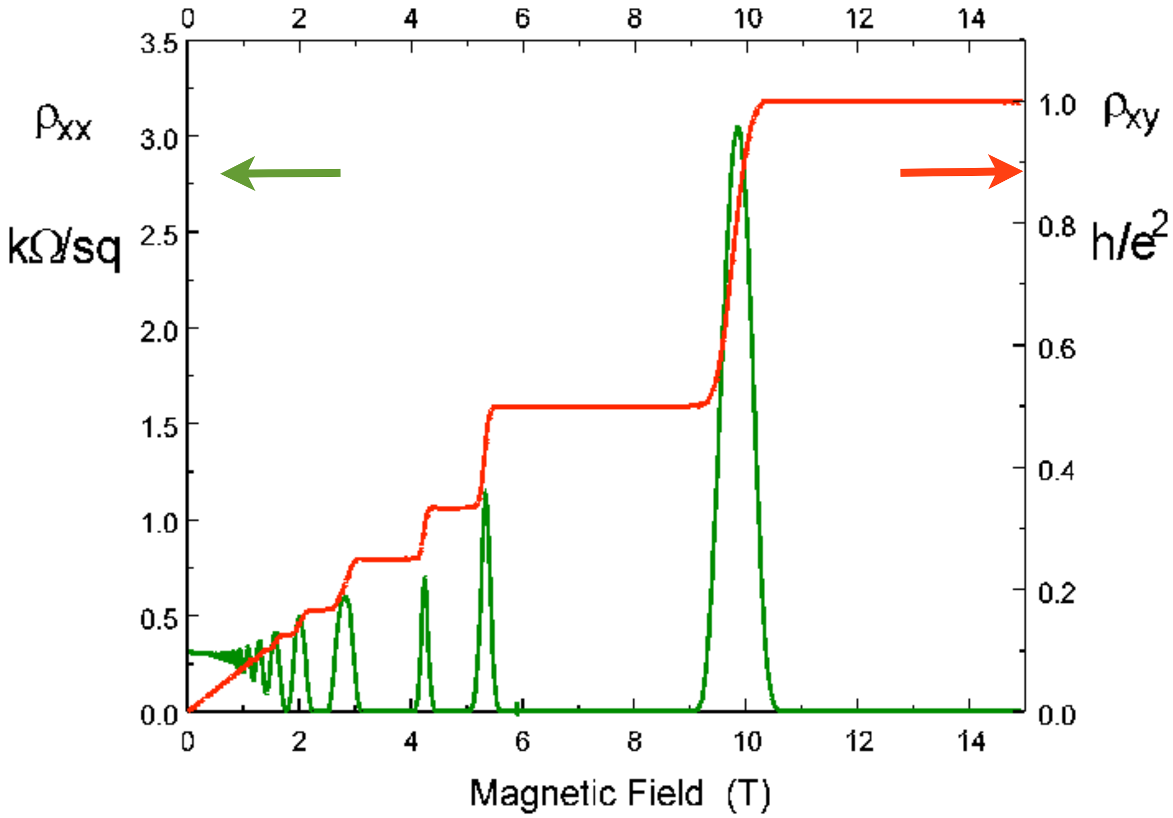
## Dirac and topological materials

More recently, physicists have gone beyond the paradigm of broken symmetries to find new states of matter with non-trivial topology



# In 1982, Von Klitzing discovered that the Hall conductivity in bad metals is exactly quantized in 2D

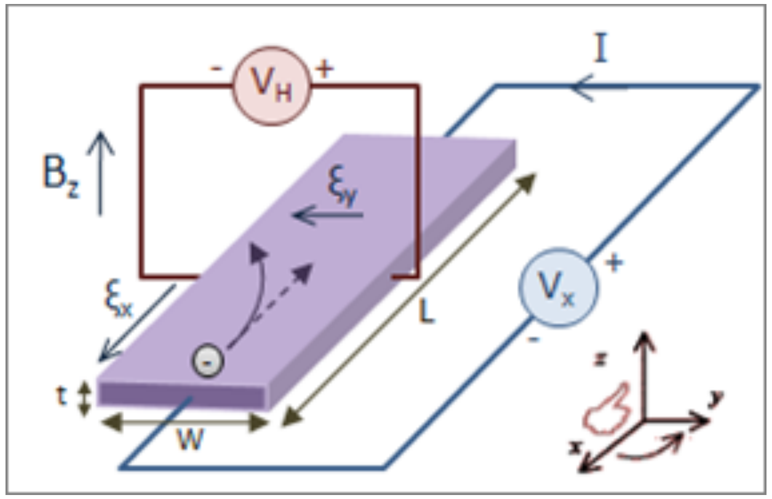
The Nobel Prize in Physics 1985 was awarded to Klaus von Klitzing *"for the discovery of the quantized Hall effect".*




$$\sigma_{xy} = n\frac{e^2}{h}$$

Integer

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}$$



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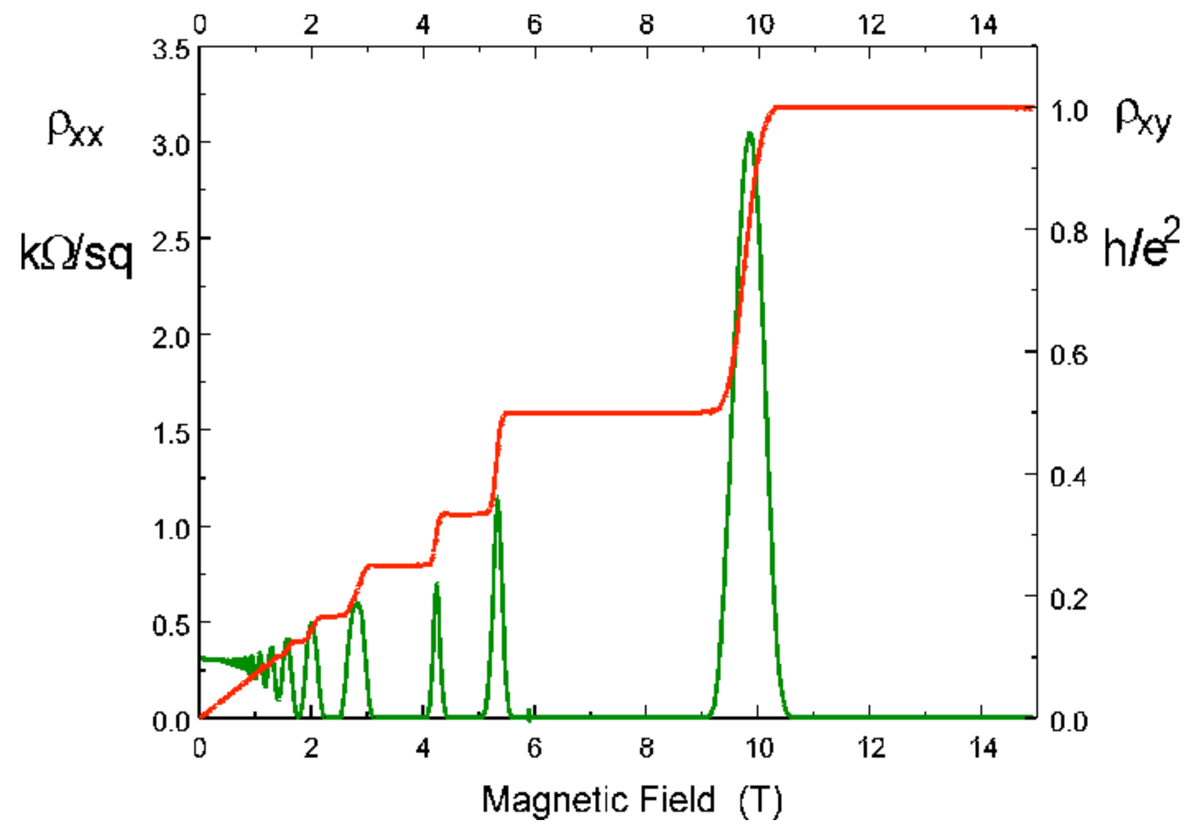


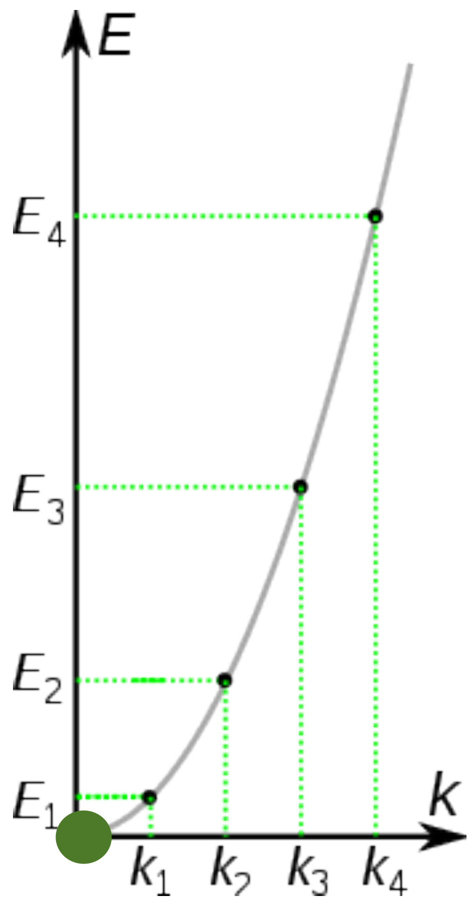

$$\sigma_{xy} = n\frac{e^2}{h}$$

Integer

Subsequent measurements confirmed the quantization in steps of $e^2/h$ with an accuracy of $10^{-9}$ !

Why is the quantization so good?

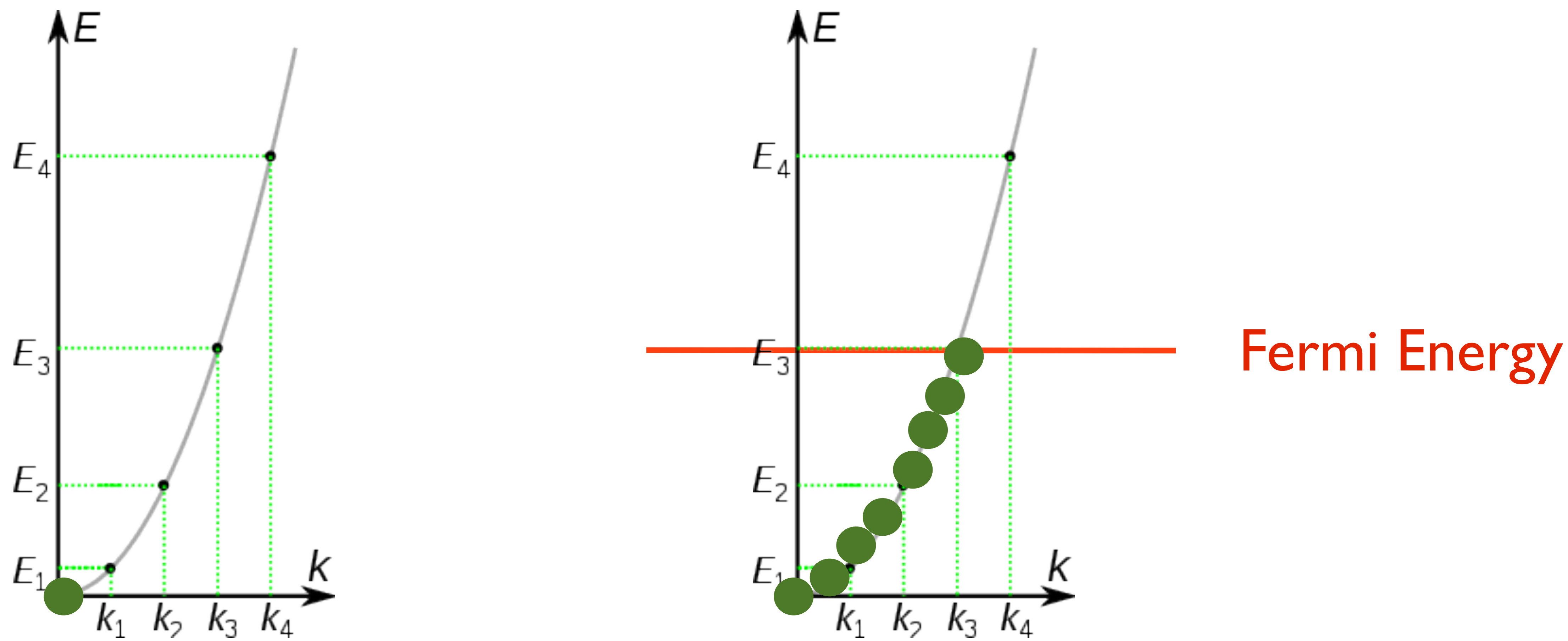
In galilean invariant systems (non-relativistic), the energy of a particle is proportional to the square of the momentum




In the ground state, a single free electron is at rest (k=0)

$$E = \frac{\hbar^2 k^2}{2m}$$

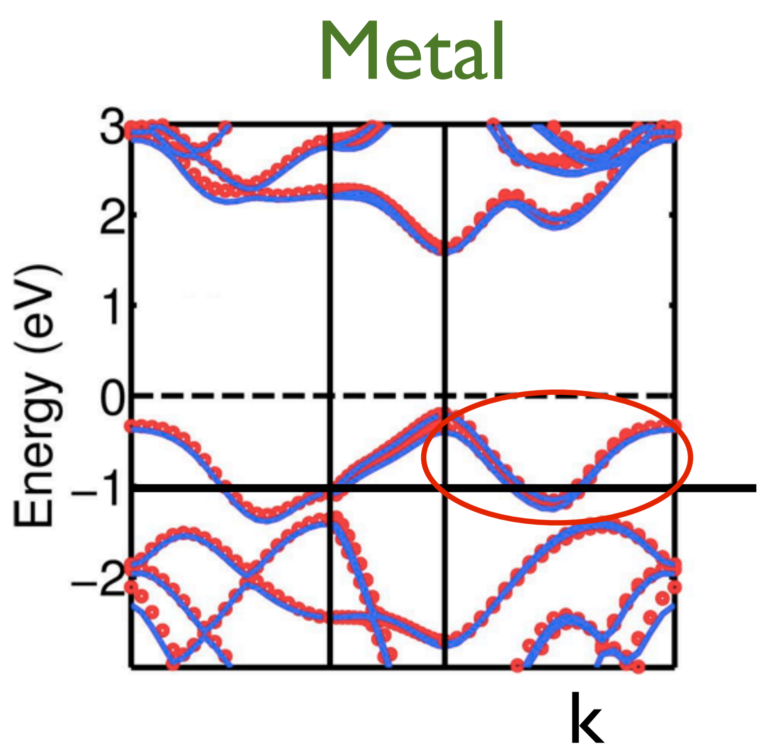
In galilean invariant systems (non-relativistic), the energy of a particle is proportional to the square of the momentum



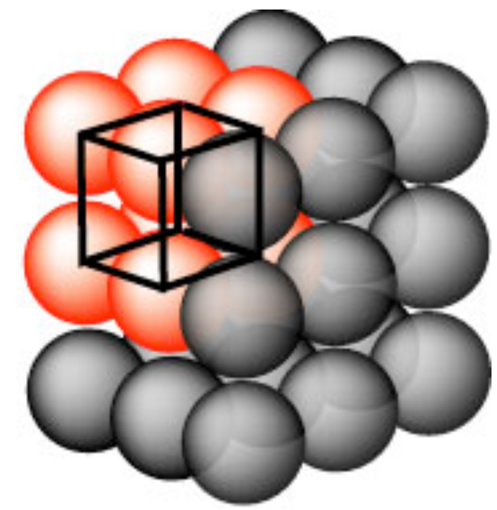

Because of Pauli principle, two electrons cannot occupy the same quantum state.

If one adds many free electrons, the states below the Fermi level are occupied and the ones above it are empty.

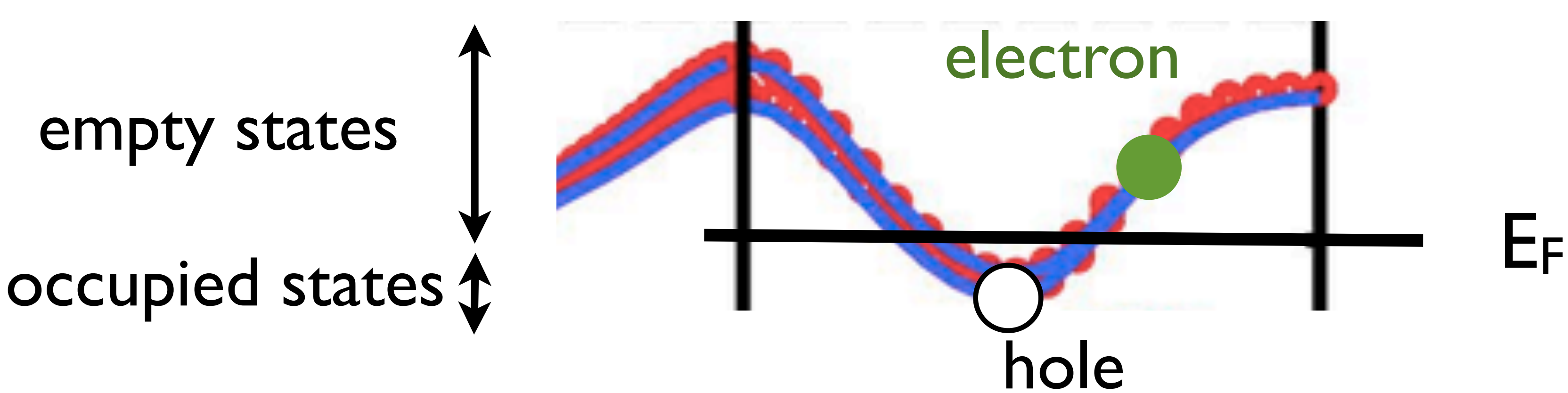
In solids (periodic potential), the energy spectrum of electrons can be quite complicated




Fermi Energy ($E_F$)

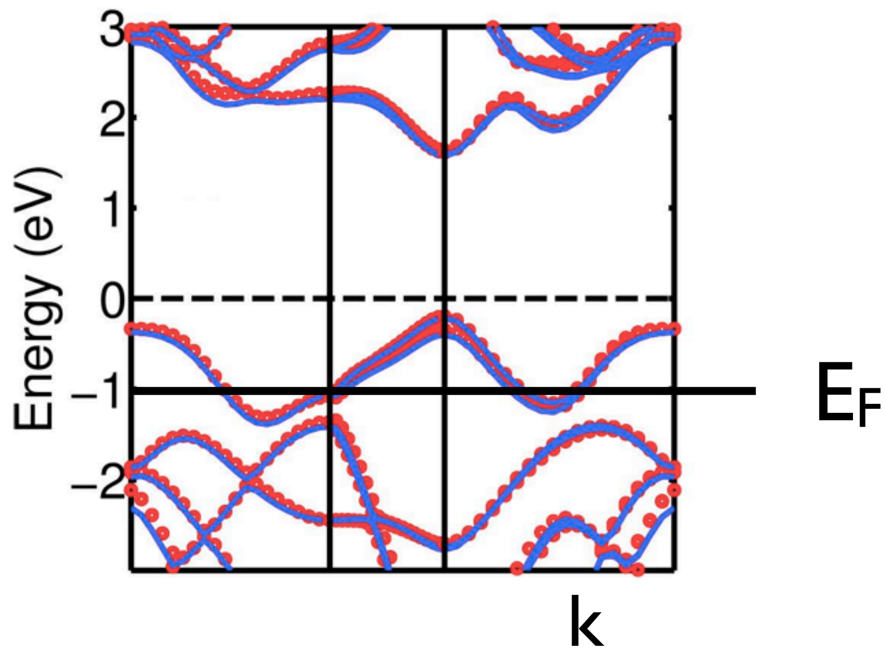


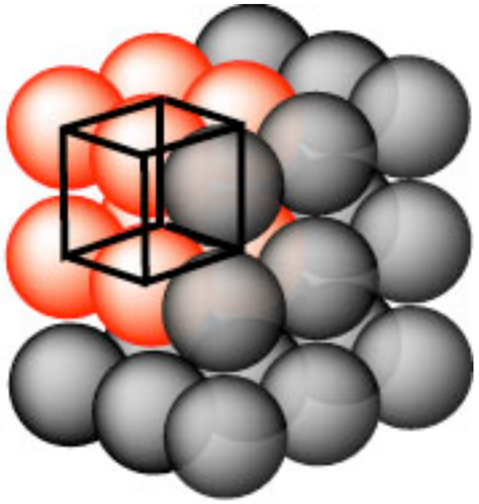
If the Fermi level crosses the electronic bands, the highest occupied state can be easily excited by a bias voltage (metallic state)



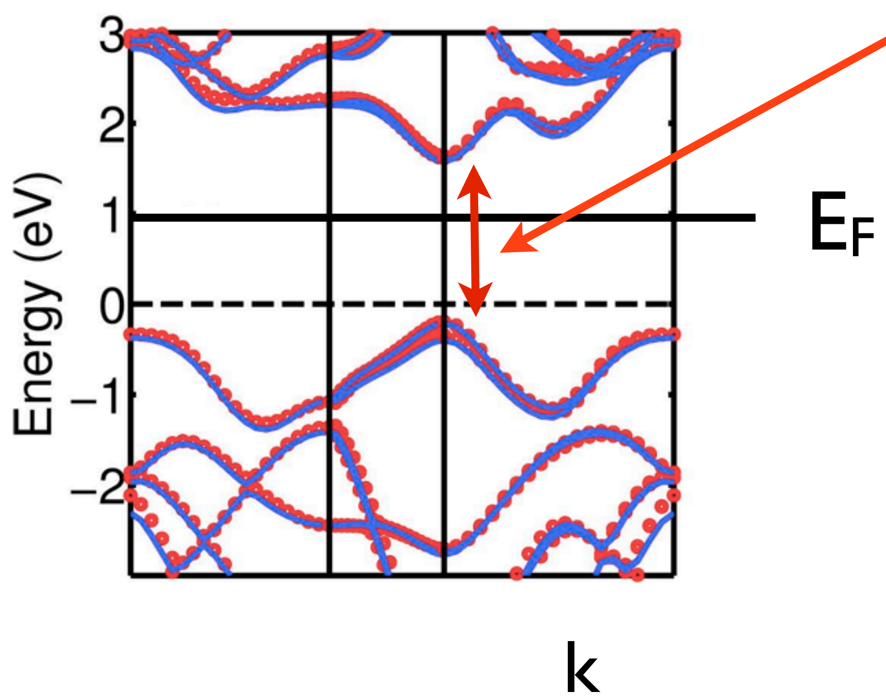
In solids (periodic potential), the energy spectrum of electrons can be quite complicated

Metal



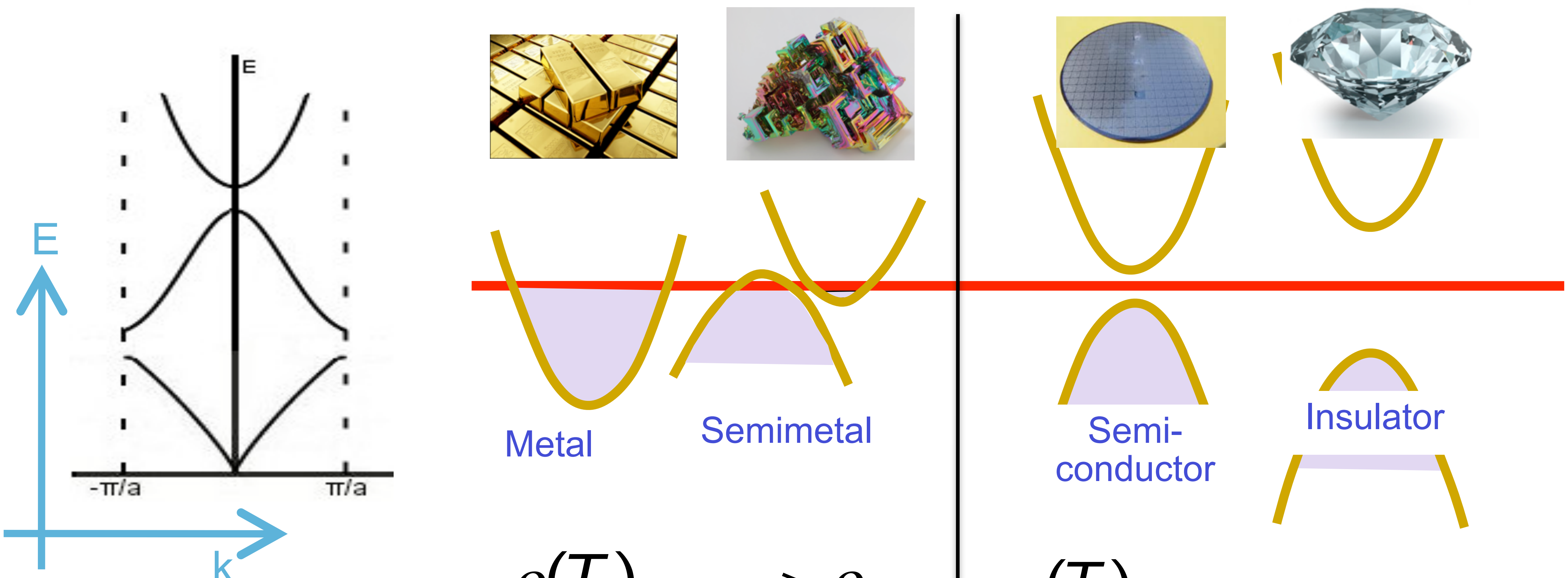



Band Gap




If the Fermi energy lives inside the band gap, the electrons cannot be easily excited with a bias voltage (insulating behavior)

# Band Structure: Conductors and Insulators




$$\rho(T)_{T \to 0} \to \rho_0 \qquad \rho(T)_{T \to 0} \to \infty$$

There is a new class of materials that does not fit in this classification: topological materials!

Topology is a field of mathematics concerned with properties that remain invariant under continuous deformations


## Topological index and invariants

$$\chi = 2(1 - g)$$

# of handles

$$\chi = \frac{1}{2\pi} \iint K \mathrm{d}S$$

Gaussian curvature

Integer

# Gaussian curvature

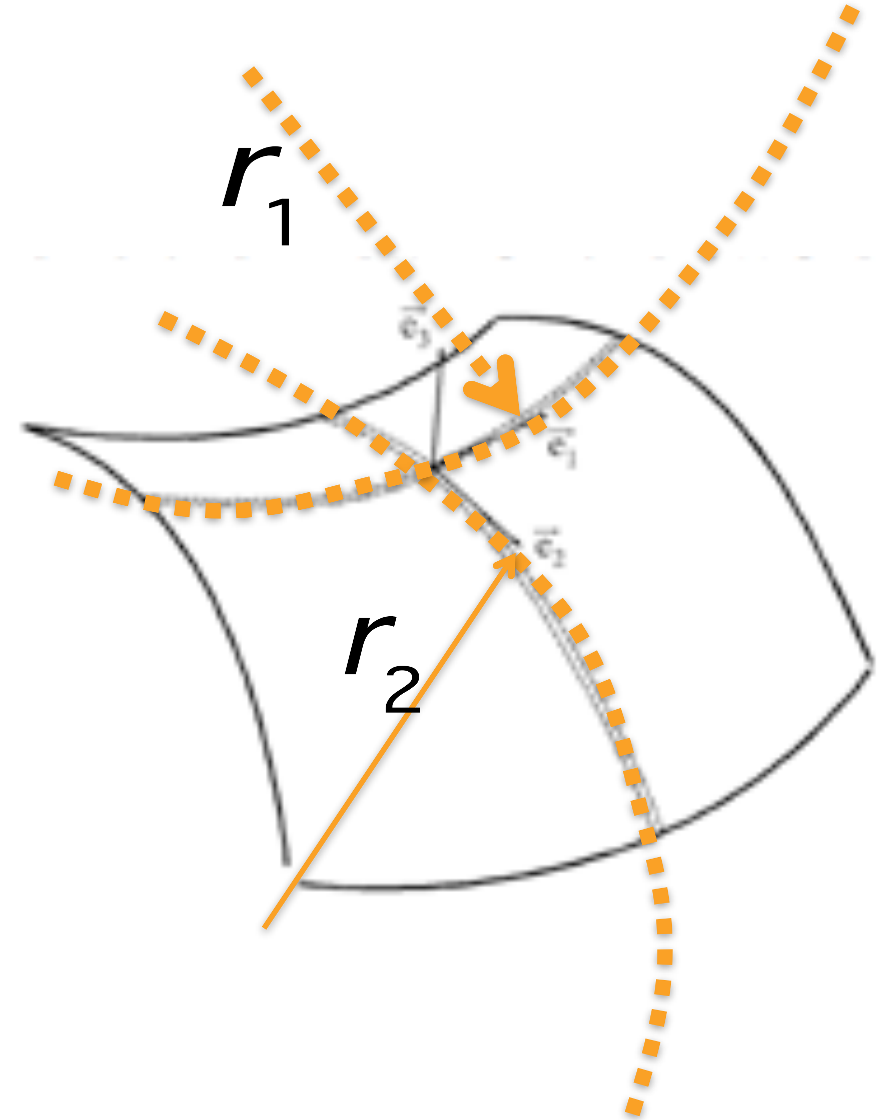
$$K = \kappa_1 \kappa_2$$

maximum curvature

minimum curvature

$$\kappa_{1,2} = \frac{1}{r_{1,2}}$$

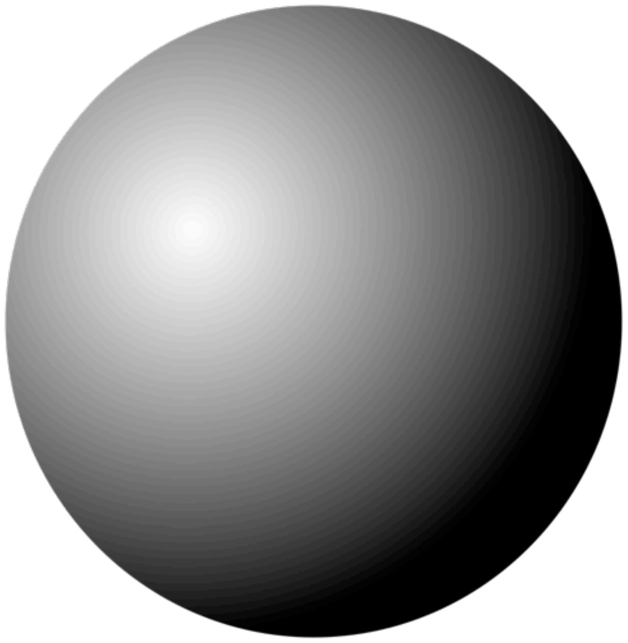
radius of curvature




$$\chi = \frac{1}{2\pi} \iint K \, \mathrm{d}S$$

Topological invariant

# Gaussian curvature (sphere)



$$K = \kappa_1 \kappa_2$$

minimum curvature ($\kappa_1$), maximum curvature ($\kappa_2$)

$$Area = 4\pi r^2$$

$$K = \frac{1}{r^2}$$

$$\kappa_{1,2} = \frac{1}{r_{1,2}}$$

radius of curvature ($r_{1,2}$)

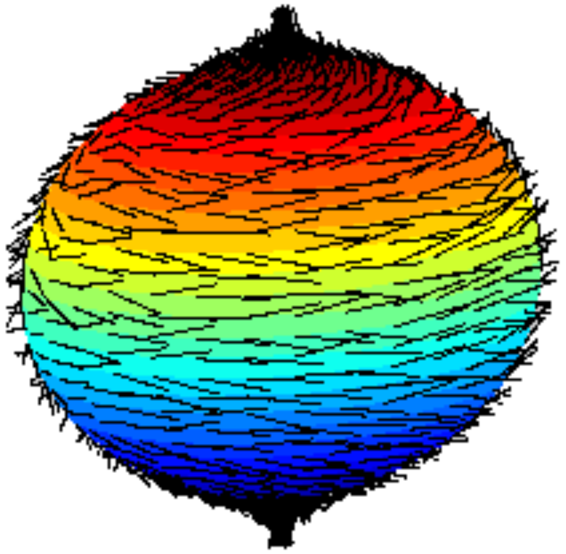
$$\chi = \frac{1}{2\pi} \iint K \mathrm{d}S$$

Topological invariant

$$\chi = \frac{1}{2\pi r^2} \int \mathrm{d}(Area) = \frac{4\pi r^2}{2\pi r^2} = 2 = 2(1-g)$$

# Hairy ball theorem

You can't comb a hairy ball without creating a cowlick.



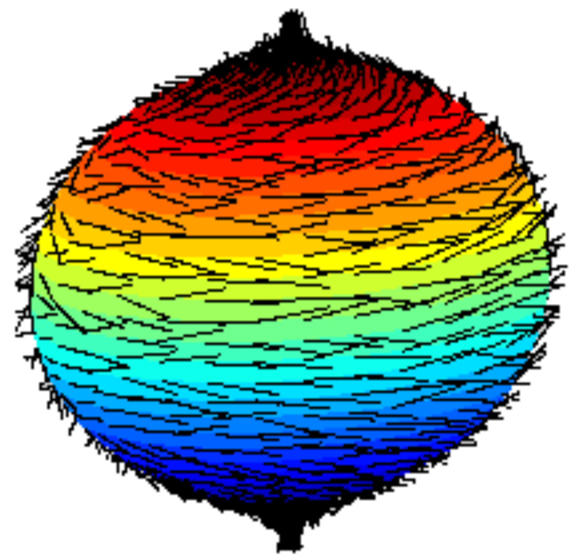
Every zero of the tangential vector field has an index. The sum of the indexes is equal to the Euler topological number

$$\chi = 2(1-g) = 2$$

Therefore a sphere has a least one zero!

# Hairy ball theorem

You can't comb a hairy ball without creating a cowlick.

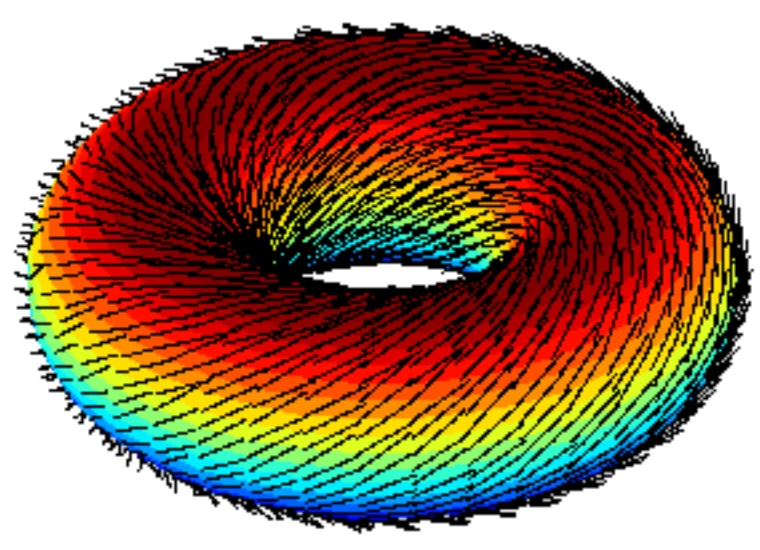


Every zero of the tangential vector field has an index. The sum of the indexes is equal to the Euler topological number.

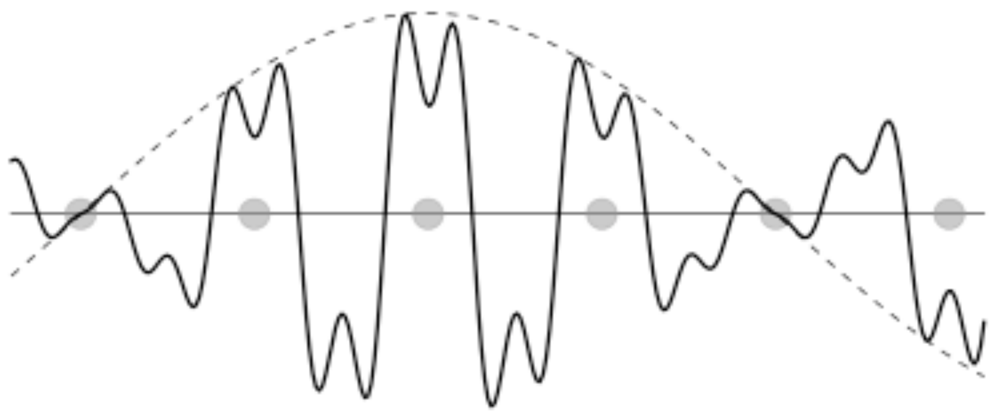
$$\chi = 2(1-g)$$

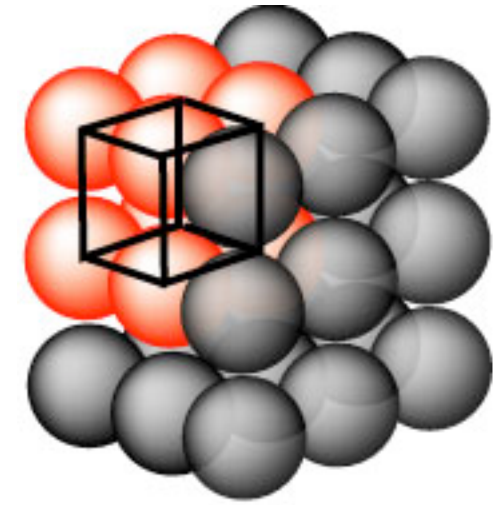
One can comb a torus without any zeros in it.

$$\chi = 2(1-g) = 0$$



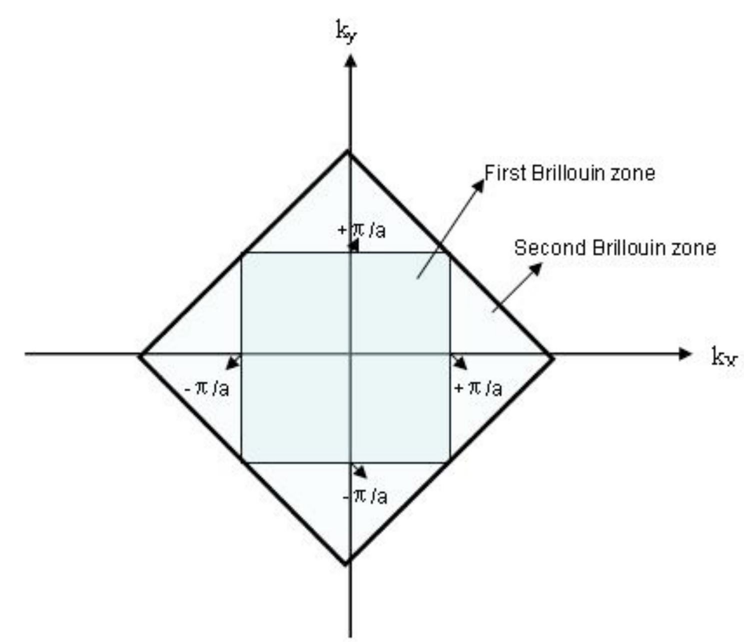
In crystals, the wavefunctions of the electrons are periodic.





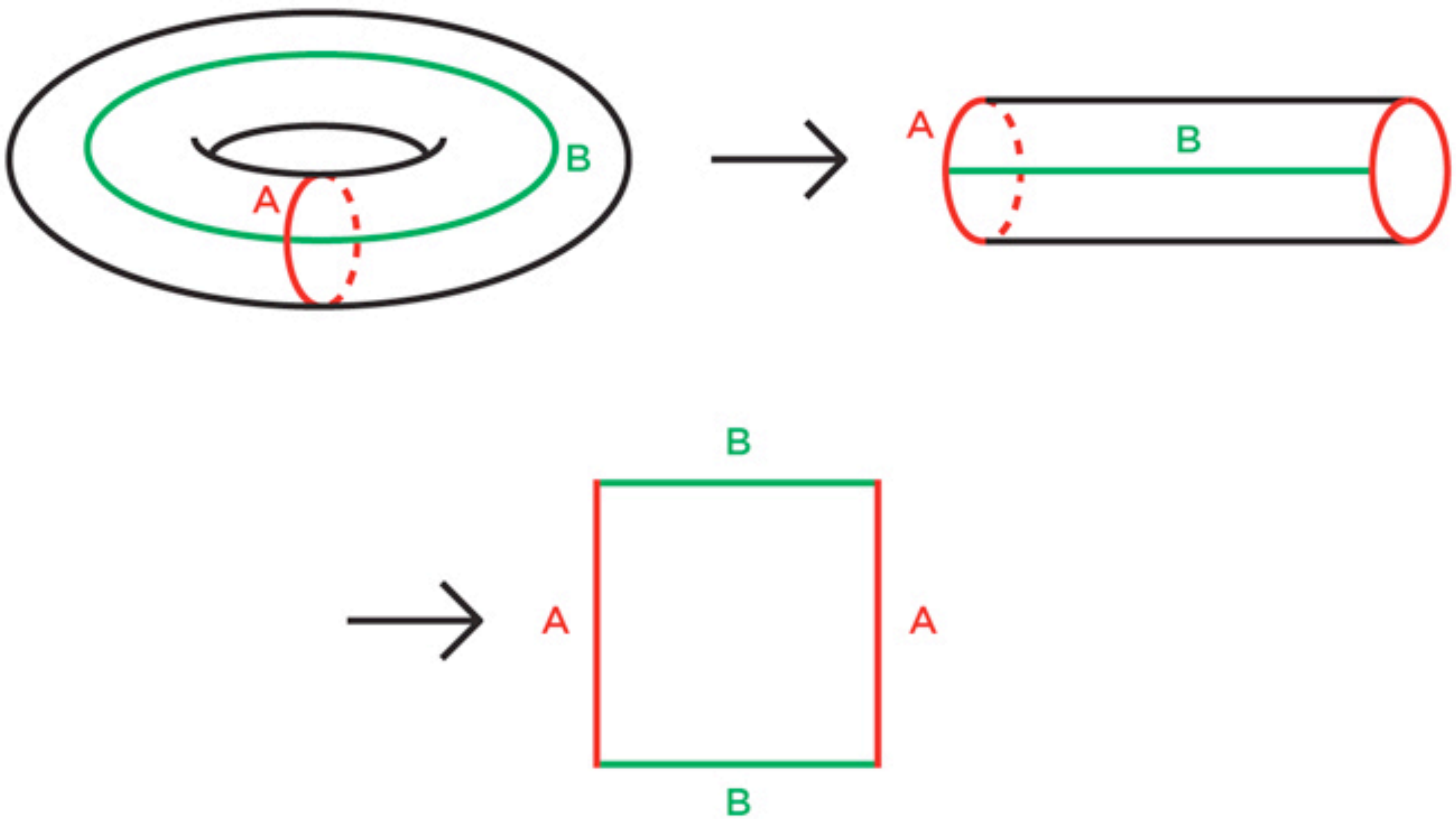
The de Broglie wavelength of the electrons must be larger than the lattice constant of the crystal.

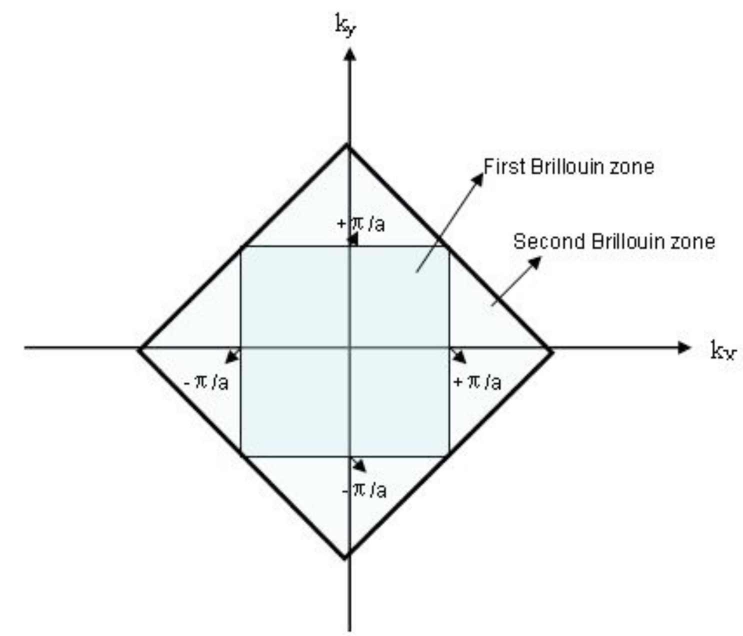
In a square lattice in 2D, the momentum of the electrons is bounded inside a square of size 1/(lattice constant)!

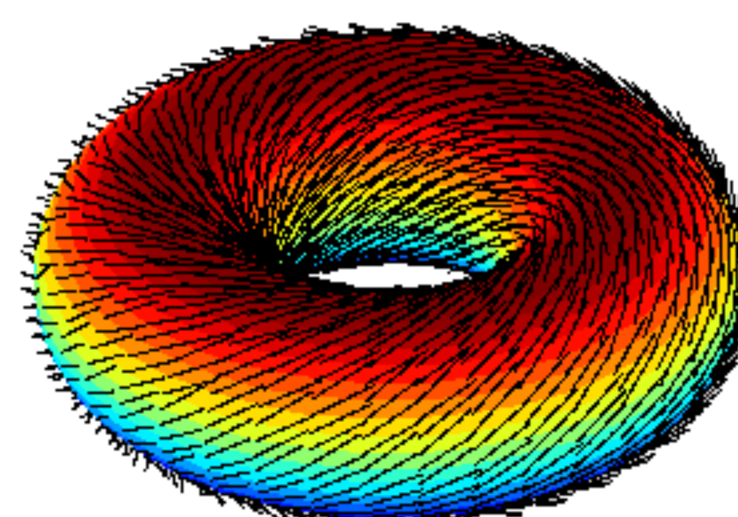


In crystals, the wavefunctions of the electrons are periodic.

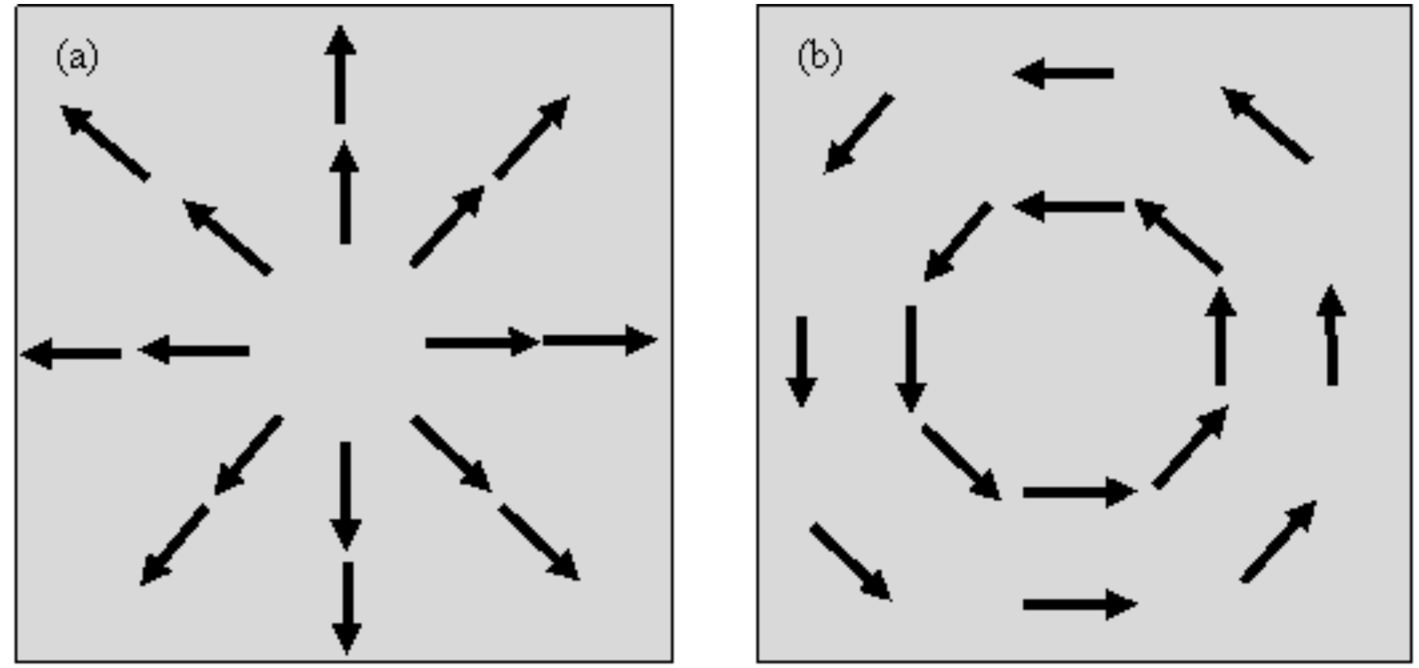
The momentum space of a periodic crystal (Brillouin zone) is homeomorphic to a torus



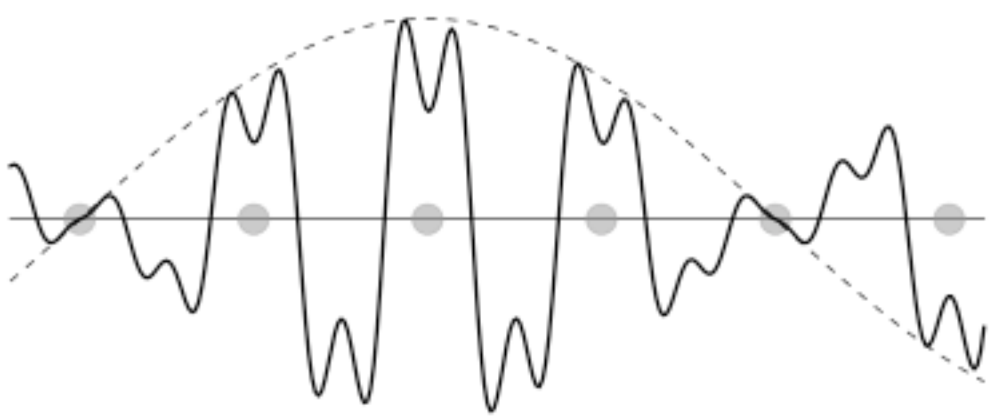



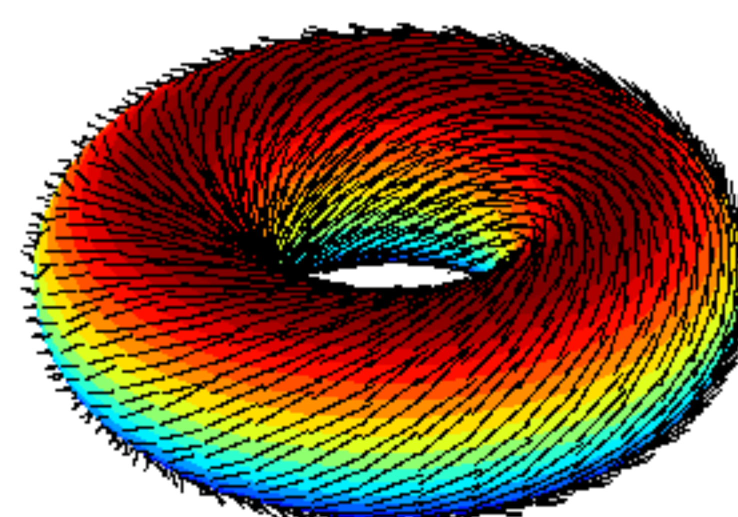
# Bloch bands




$$\psi_{n,\mathbf{k}}(\mathbf{r}) = u_{n,\mathbf{k}}(\mathbf{r})\,\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$$
$$= \langle \mathbf{r}|\psi_{n,\mathbf{k}}\rangle$$

Bloch wavefunction



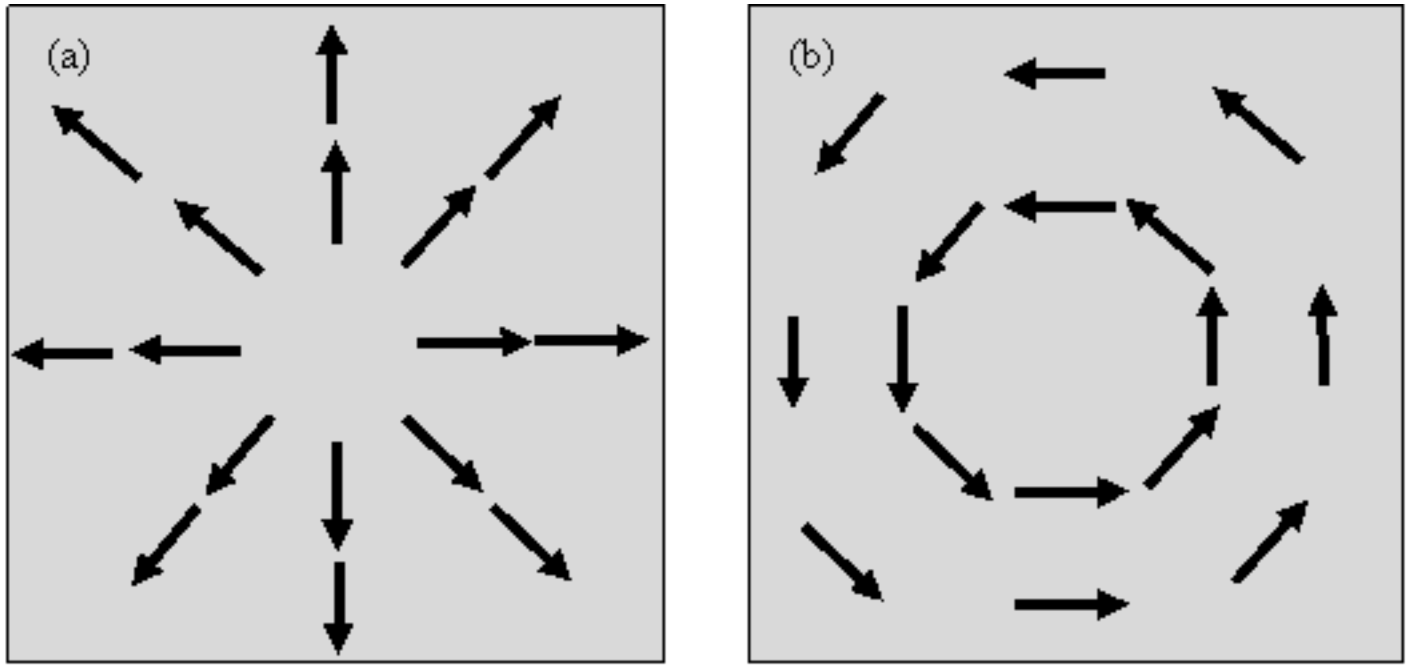


Bloch wavefunctions describe the wavefunction of the electrons in a periodic crystal.

# Bloch bands

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = u_{n,\mathbf{k}}(\mathbf{r})\,\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$$
$$= \langle \mathbf{r}|\psi_{n,\mathbf{k}}\rangle$$

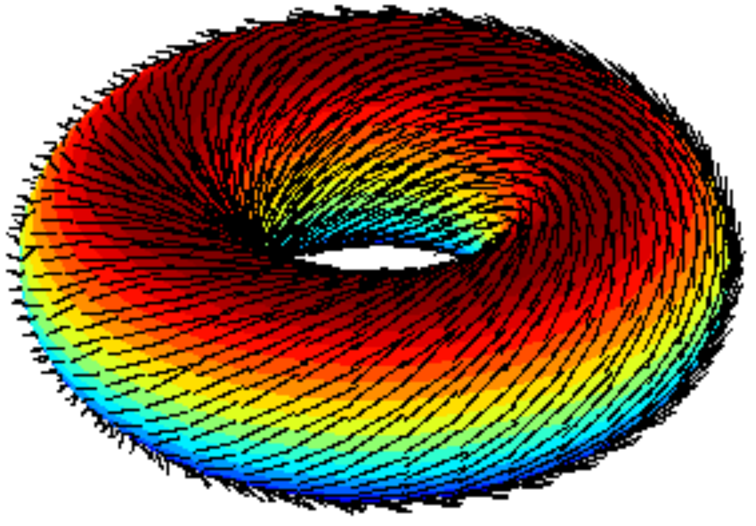
Bloch wavefunction



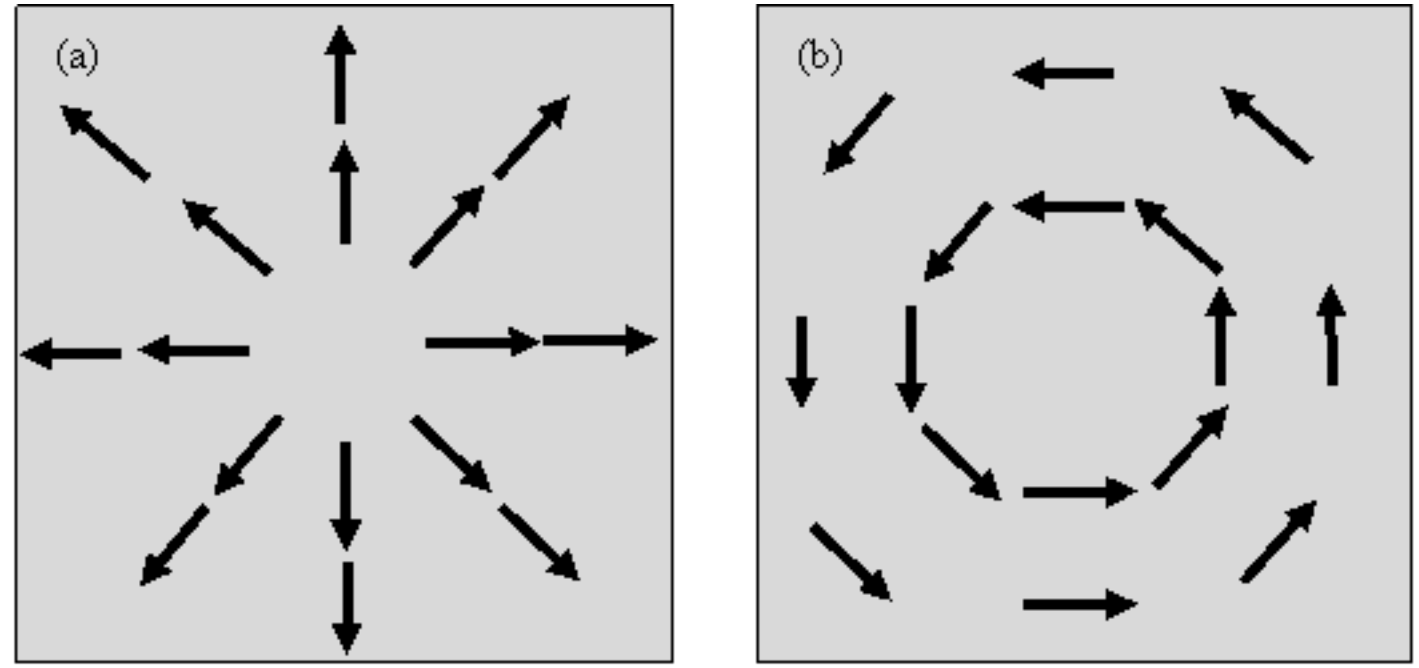

The Berry connection of the Bloch band kets, $\overbrace{i\langle\psi_{n,\mathbf{k}}|\frac{\partial}{\partial\mathbf{k}}|\psi_{n,\mathbf{k}}\rangle}^{\mathbf{A}}$

behaves as a vector field in the Brillouin zone (torus).

Loopholes or hedgehogs of the vector field have a topological index and add up to a non-zero Euler topological number in the hairy torus.



# Bloch bands




$$\psi_{n,\mathbf{k}}(\mathbf{r}) = u_{n,\mathbf{k}}(\mathbf{r})\, \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$$
$$= \langle \mathbf{r} | \psi_{n,\mathbf{k}} \rangle$$

Bloch wavefunction

$$\nu_n = \iint \mathrm{d}\mathbf{S} \cdot \nabla \times \overbrace{i\langle \psi_{n,\mathbf{k}} | \frac{\partial}{\partial \mathbf{k}} | \psi_{n,\mathbf{k}} \rangle}^{\mathbf{A}}$$

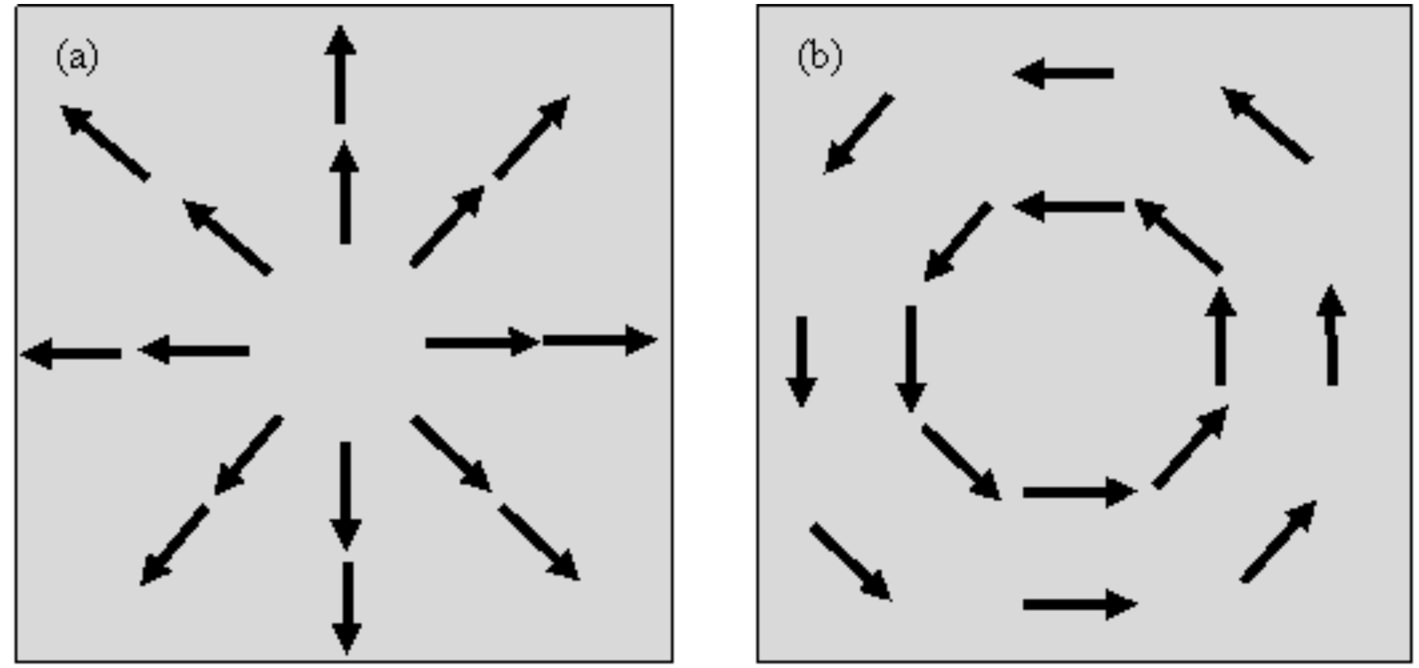
→ Berry curvature

Chern number (integer)

The Chern number is a topological invariant of Bloch bands

$$\chi = \frac{1}{2\pi} \iint K \mathrm{d}S$$

# Bloch bands

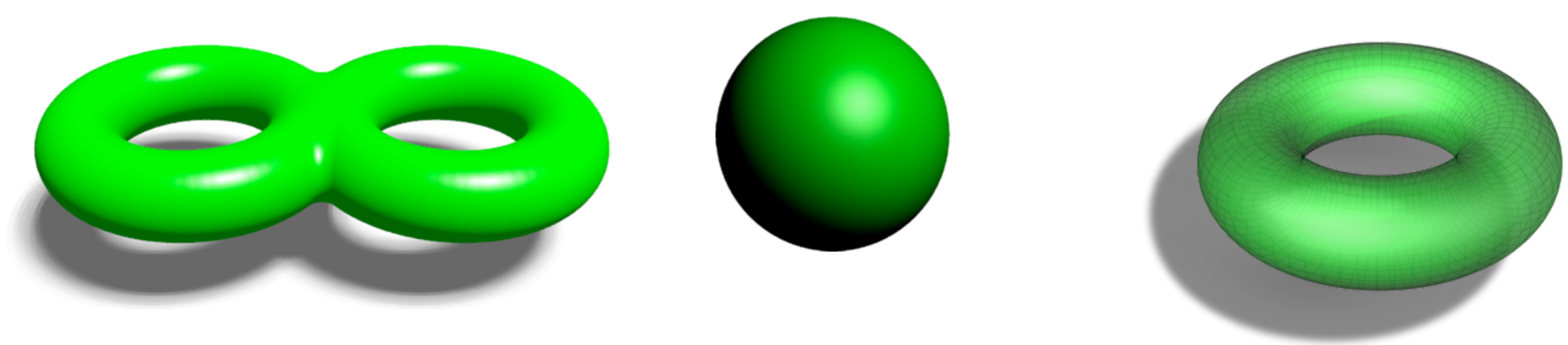



$$\psi_{n,\mathbf{k}}(\mathbf{r}) = u_{n,\mathbf{k}}(\mathbf{r})\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$$

Bloch bands

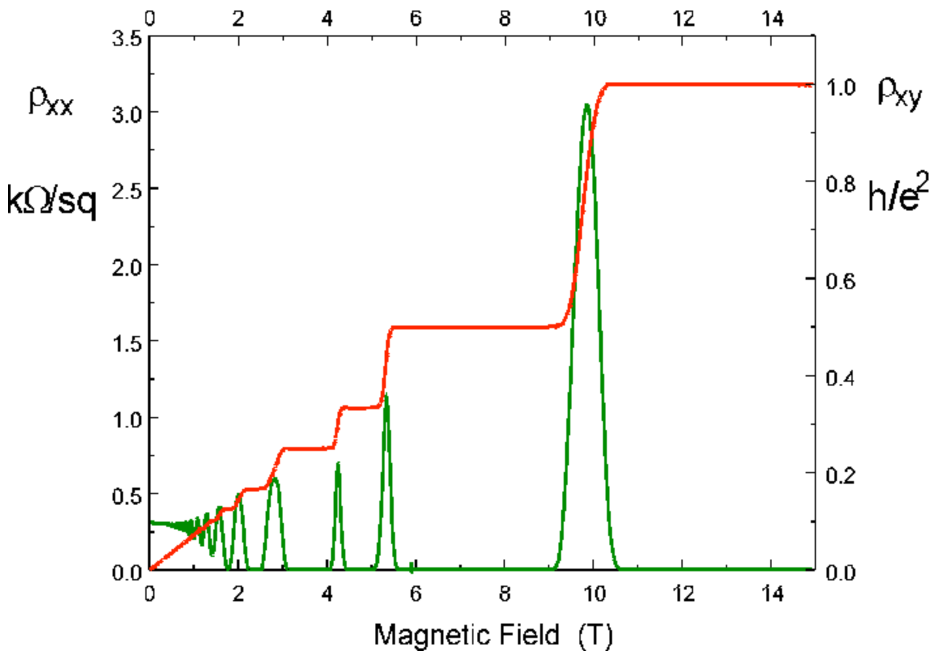
$$\nu_n = \iint \mathrm{d}\mathbf{S} \cdot \boxed{\nabla \times i\langle \psi_{n,\mathbf{k}} | \frac{\partial}{\partial \mathbf{k}} | \psi_{n,\mathbf{k}} \rangle}$$

→ Berry curvature



$$\chi = \frac{1}{2\pi} \iint K \mathrm{d}S$$

Cowlicks in the Berry curvature change the topological class of the hairy torus (Brillouin zone)!




Why is the Hall conductivity quantized?

VOLUME 49, NUMBER 6 PHYSICAL REVIEW LETTERS 9 AUGUST 1982

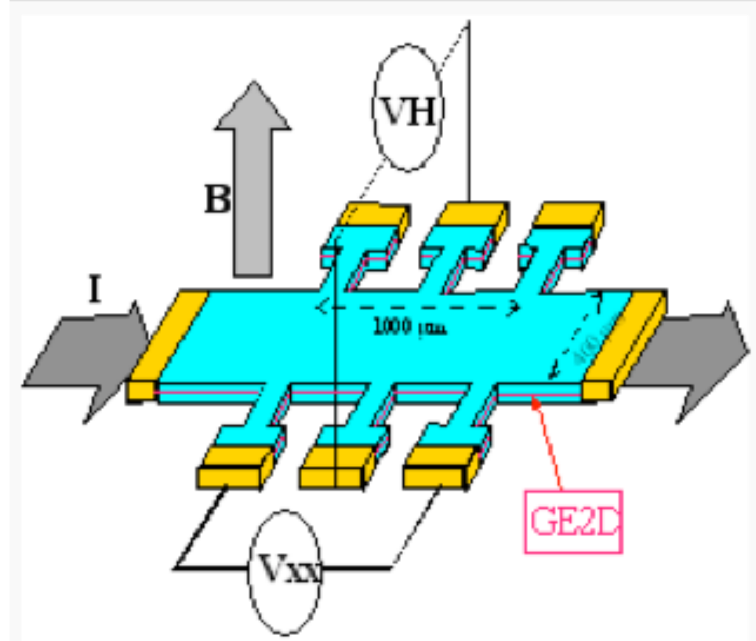
## Quantized Hall Conductance in a Two-Dimensional Periodic Potential

D. J. Thouless, M. Kohmoto,[a] M. P. Nightingale, and M. den Nijs
*Department of Physics, University of Washington, Seattle, Washington 98195*
(Received 30 April 1982)

The Hall conductance of a two-dimensional electron gas has been studied in a uniform magnetic field and a periodic substrate potential $U$. The Kubo formula is written in a form that makes apparent the quantization when the Fermi energy lies in a gap. Explicit expressions have been obtained for the Hall conductance for both large and small $U/\hbar\omega_c$.

$$\nu_n = \iint \mathrm{d}\mathbf{S} \cdot \nabla \times i\langle \psi_{n,\mathbf{k}} | \frac{\partial}{\partial \mathbf{k}} | \psi_{n,\mathbf{k}} \rangle$$

$$\sigma_{xy} = \frac{e^2}{h} \sum_n \nu_n$$

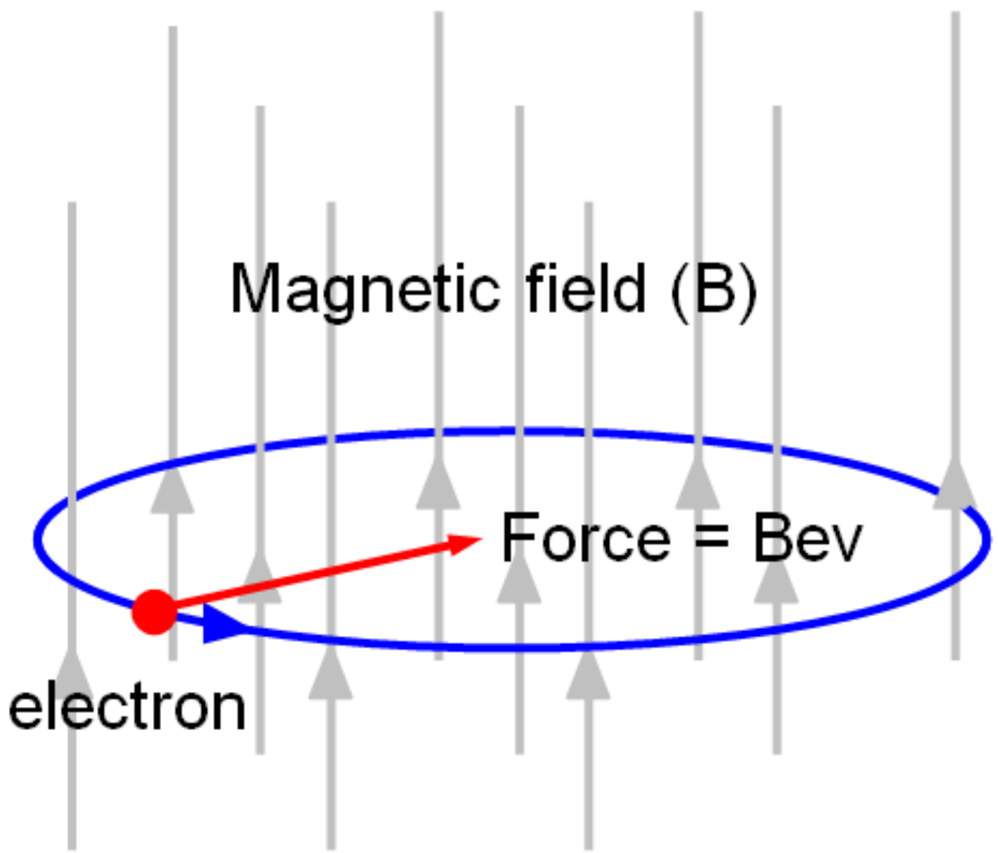


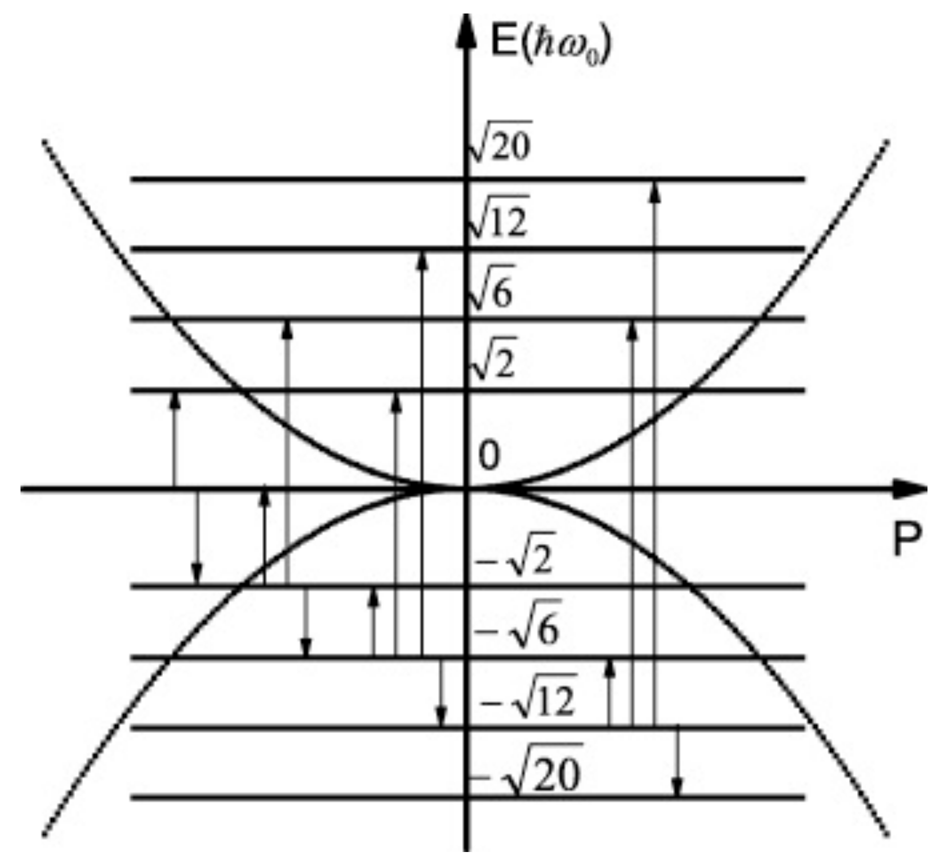

two-dimensional electron gas
with Hall bar geometry

Quantum hall conductivity is quantized by the Chern number!

# Topological matter

In 2D, electrons move in cyclotron orbits in the presence of a magnetic field

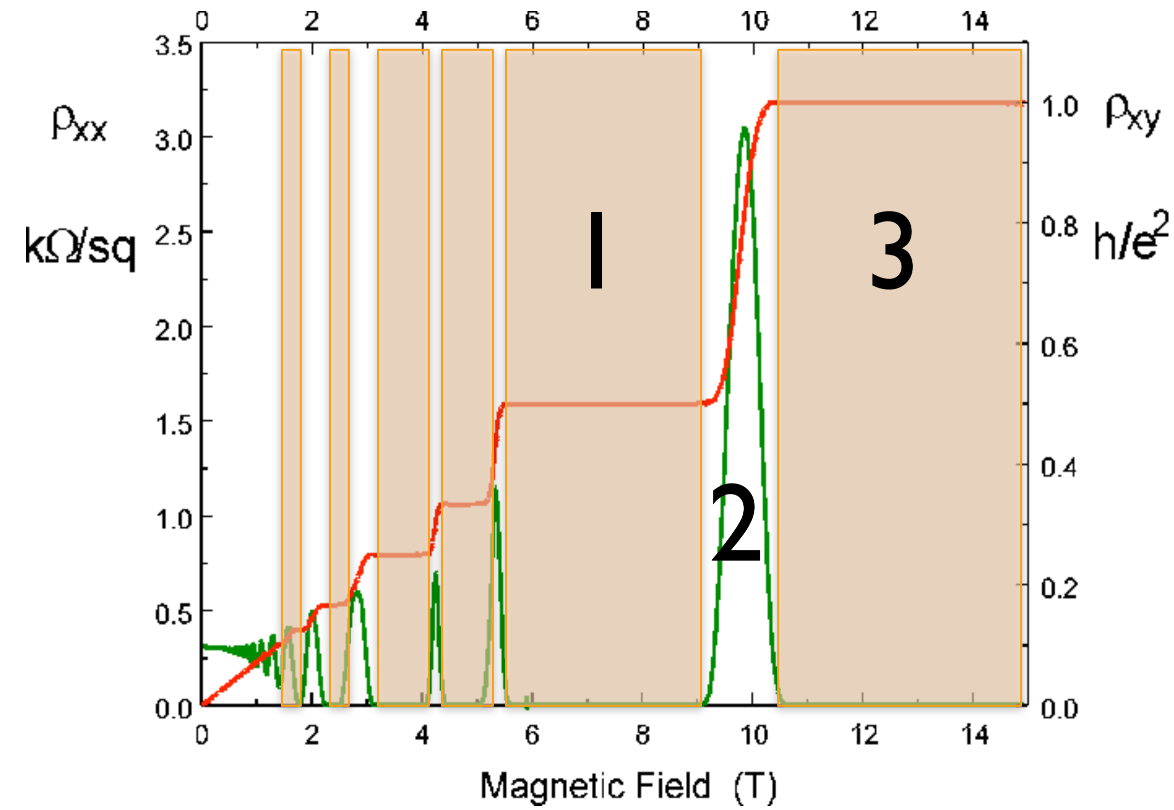


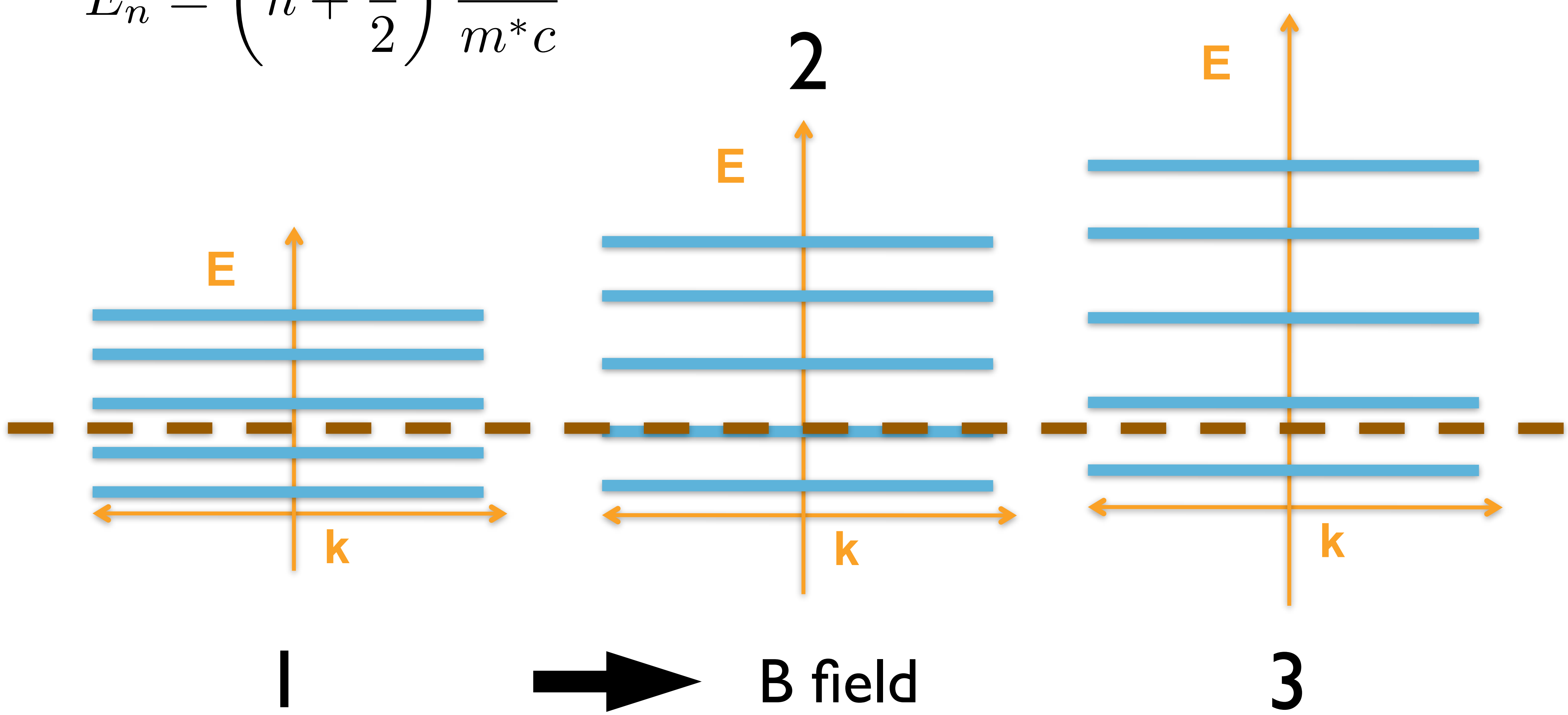

Due to quantum interference, only a discrete number of wavelengths are allowed (Landau energy levels)

# Integer quantum Hall effect

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}$$

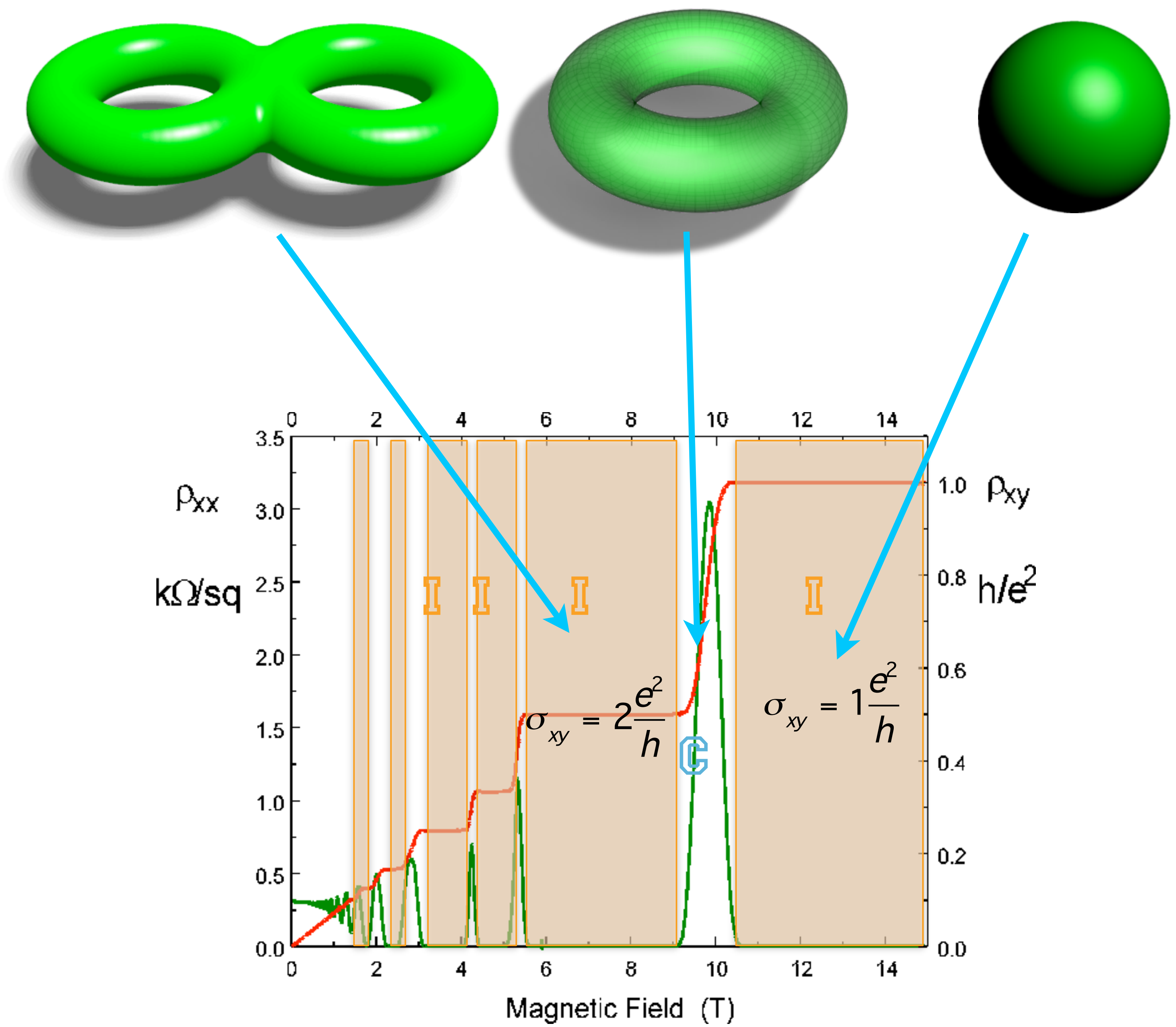



$$E_n = \left(n + \frac{1}{2}\right)\frac{heB}{m^*c}$$



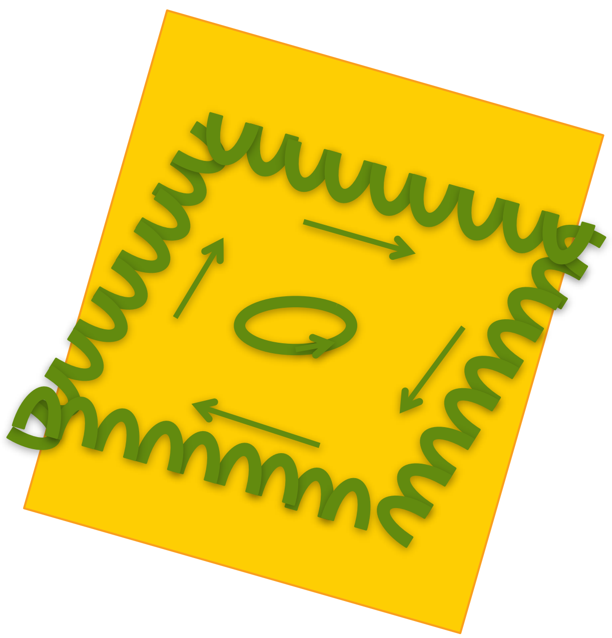
# Quantum Hall conductivity is quantized by the Chern number

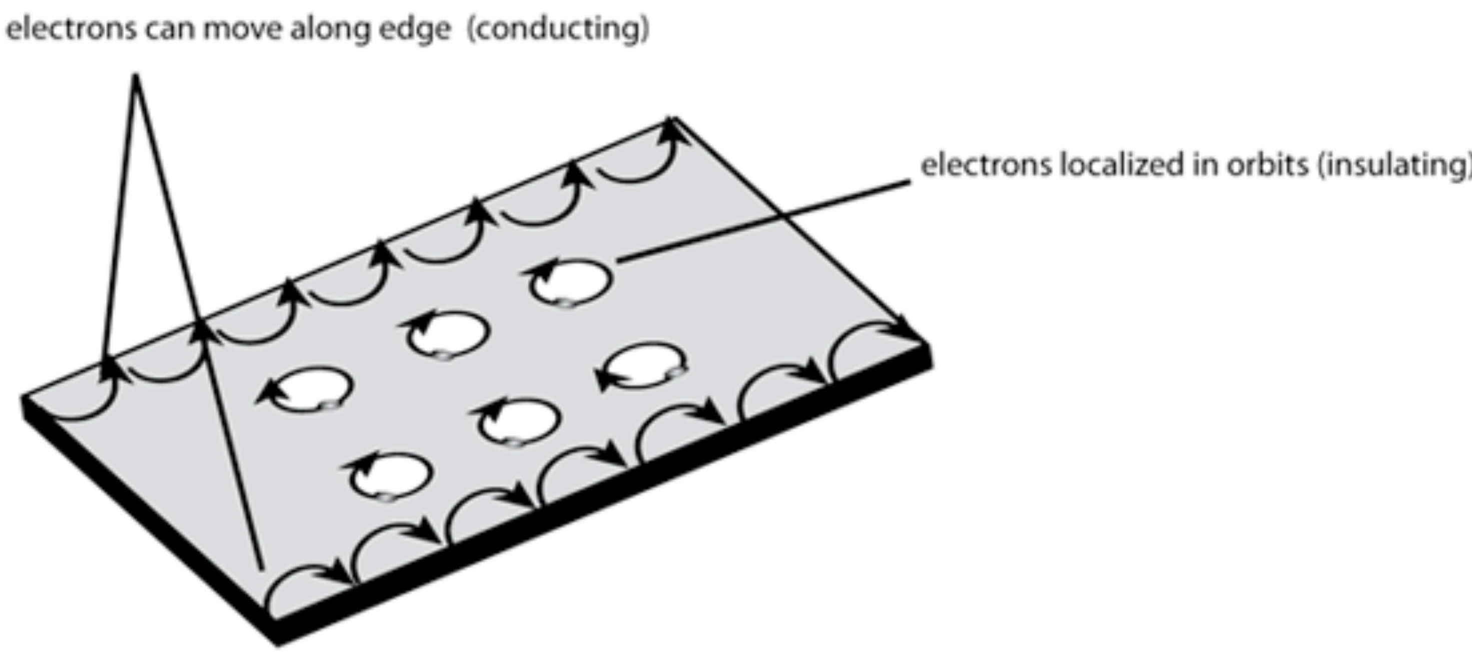
$$\sigma_{xy} = \frac{e^2}{h}\sum_n \nu_n$$



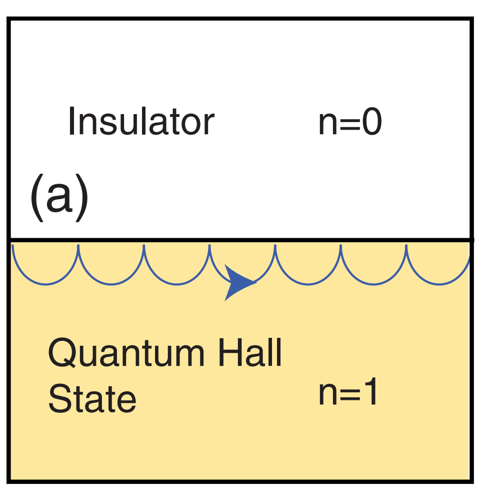

**Topologically distinct insulating phases**

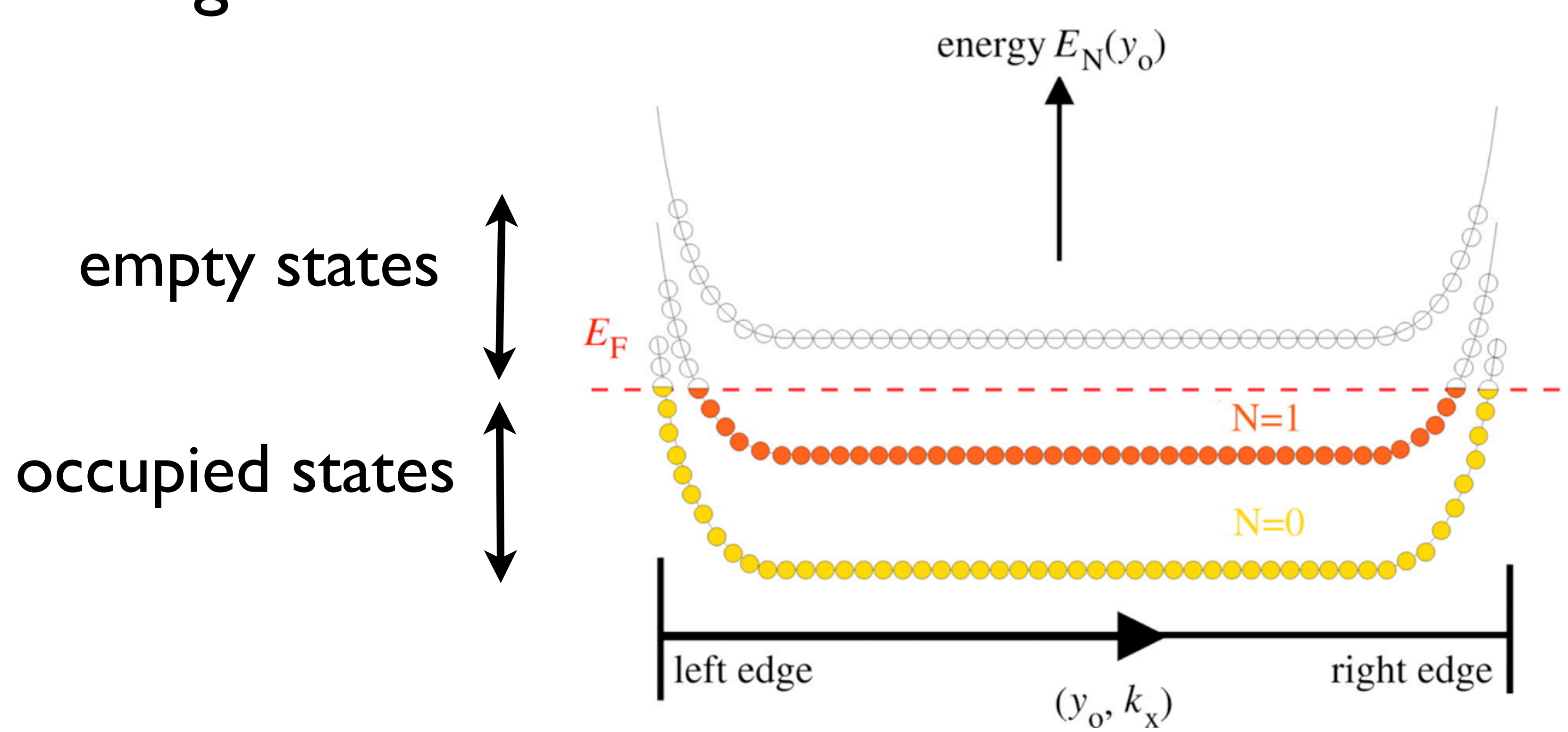
# Bulk-Boundary Correspondence





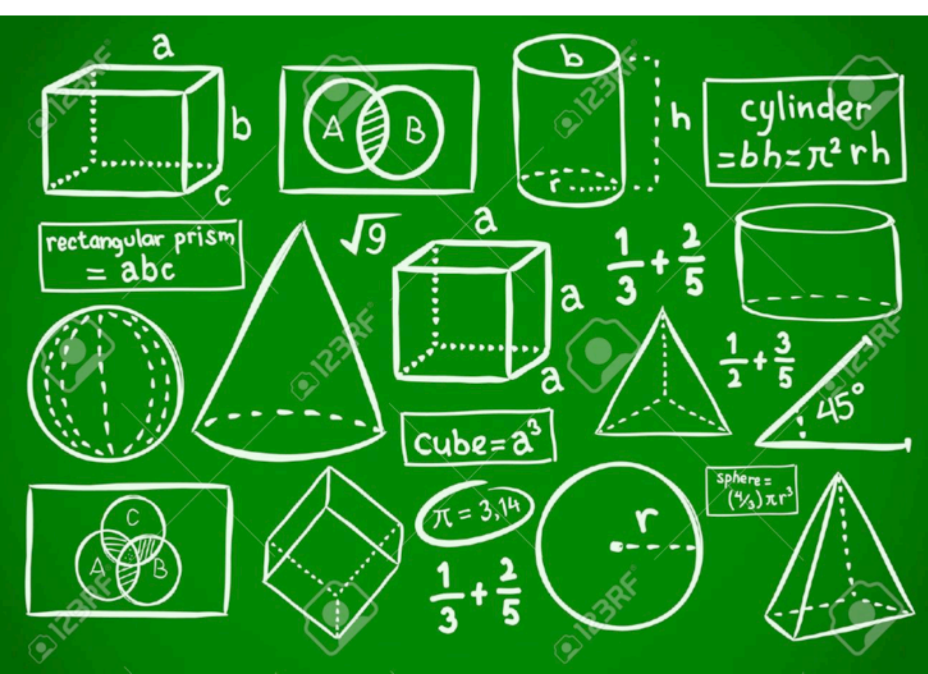

Hall conductivity is quantized by the number of 1D channels at the edge!

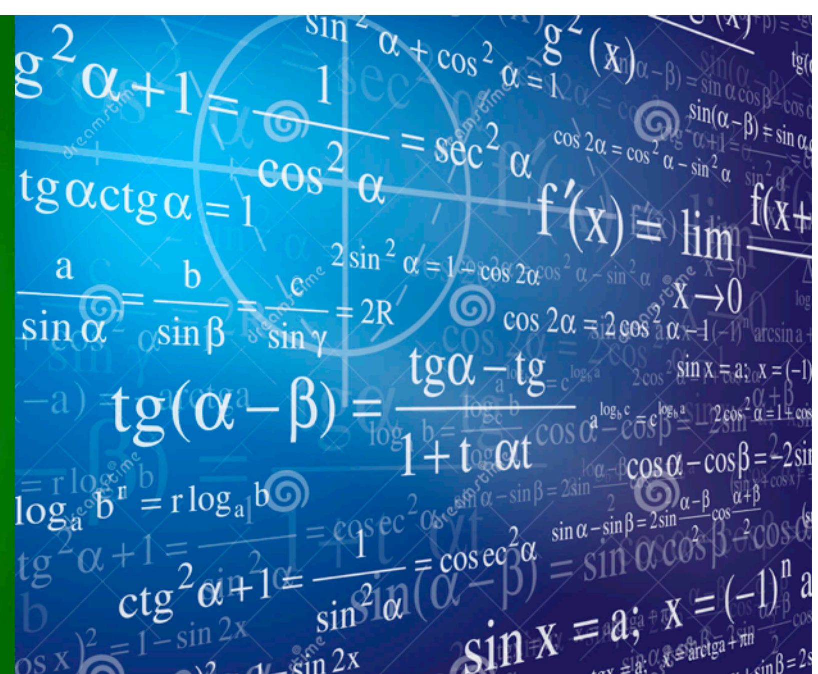


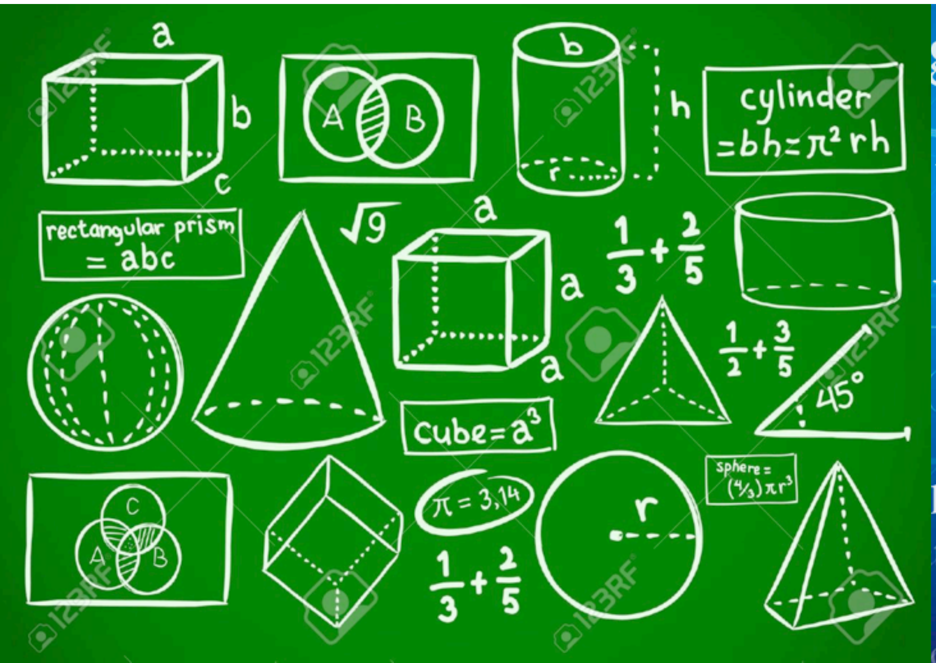
Lesson I: Some concepts appear to be pure mathematical abstractions until they lead the way to understanding new fundamental discoveries.

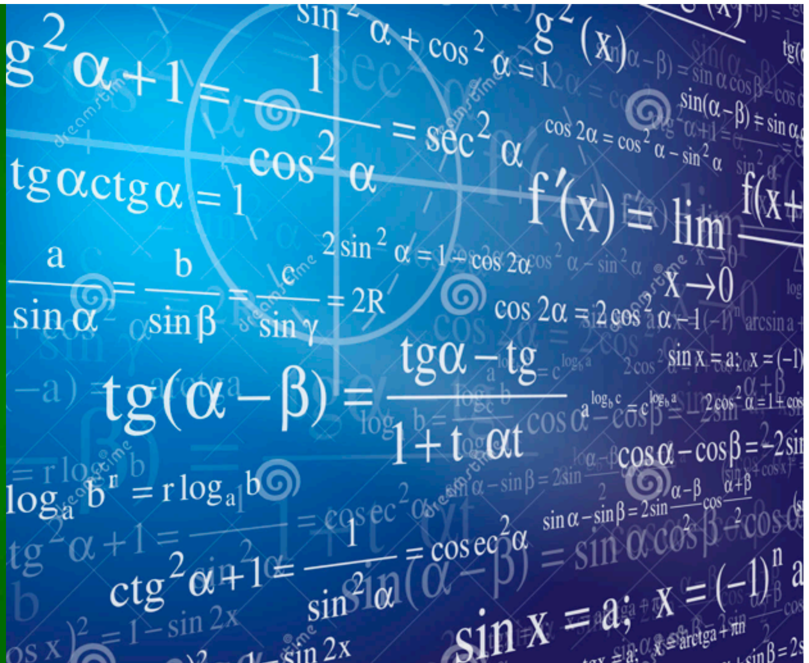
Try to learn the language, even if you would like to become an experimentalist!



There are other classes of materials that also have unusual topological properties in the absence of a magnetic field.



In 1928, Paul Dirac proposed a relativistic wave equation for spin 1/2 particles, such as electrons and quarks.

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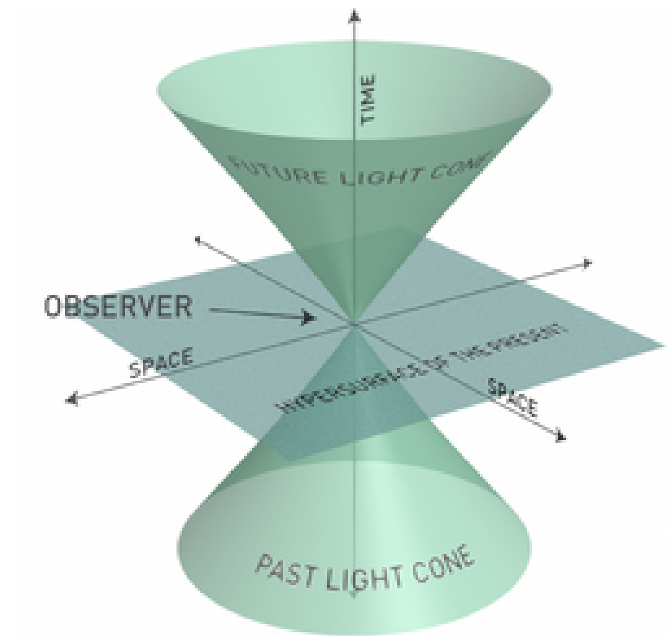


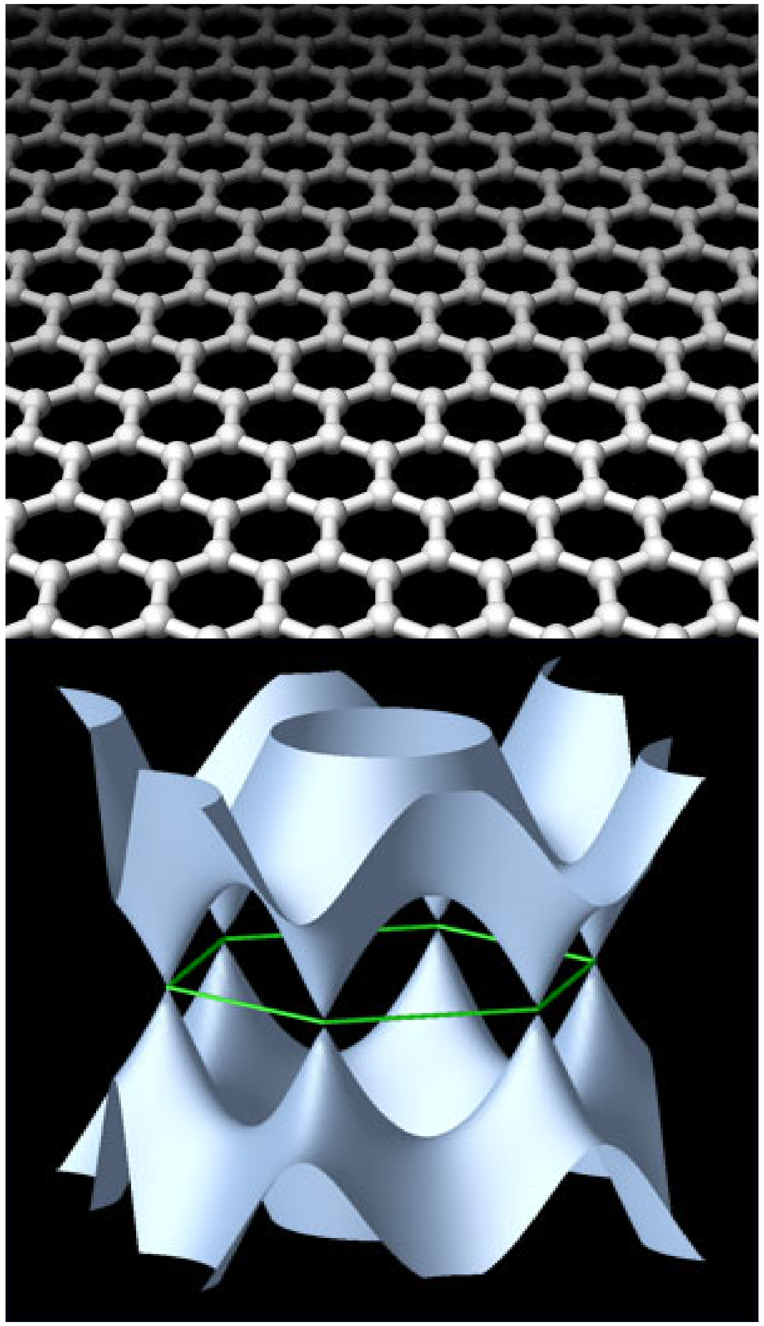

In the massless case, fermions follow a Dirac equation with chiral states

$$E(p) = \pm v\, p$$

$$H\,\Psi_\pm = v\begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}\Psi_\pm = v\,\vec{\sigma}\cdot\mathbf{p}\Psi_\pm = \pm vp\Psi_\pm$$

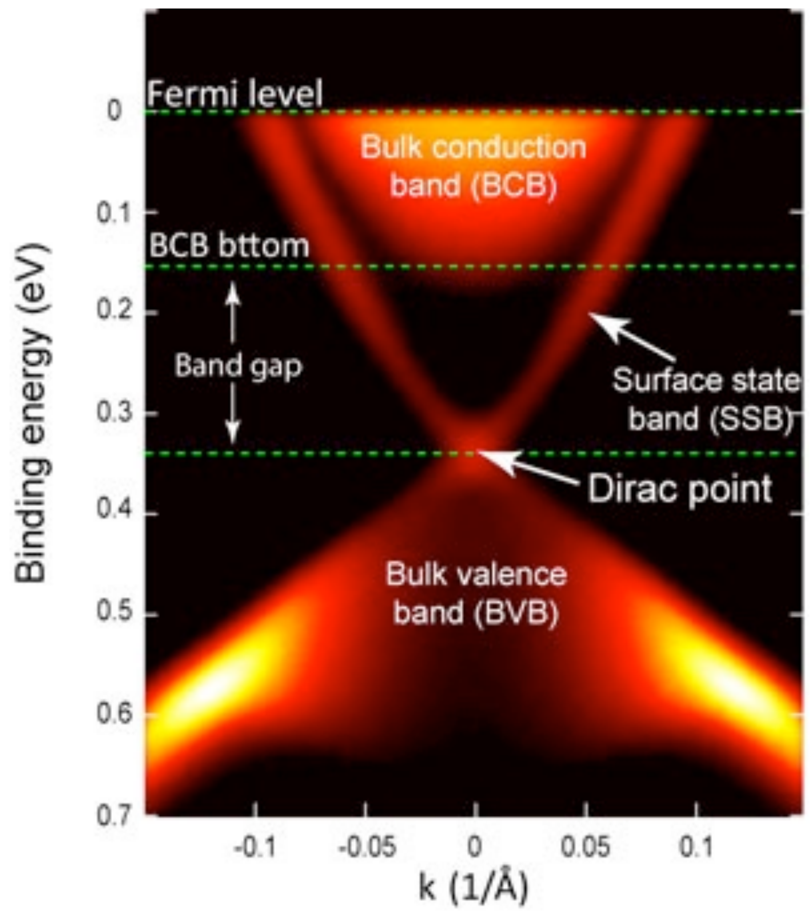
momentum operator

# Dirac materials

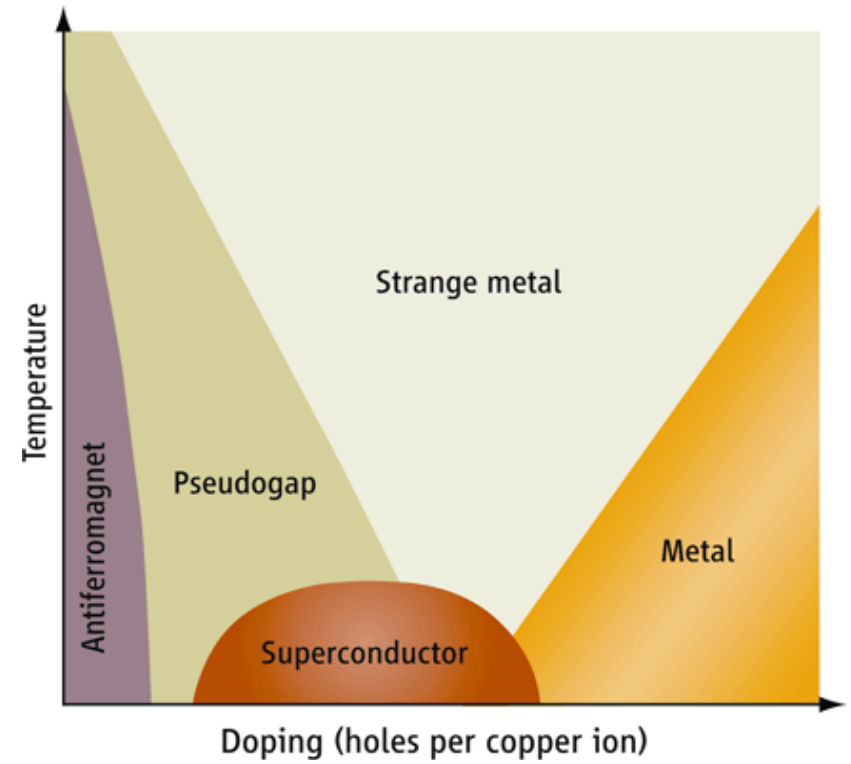


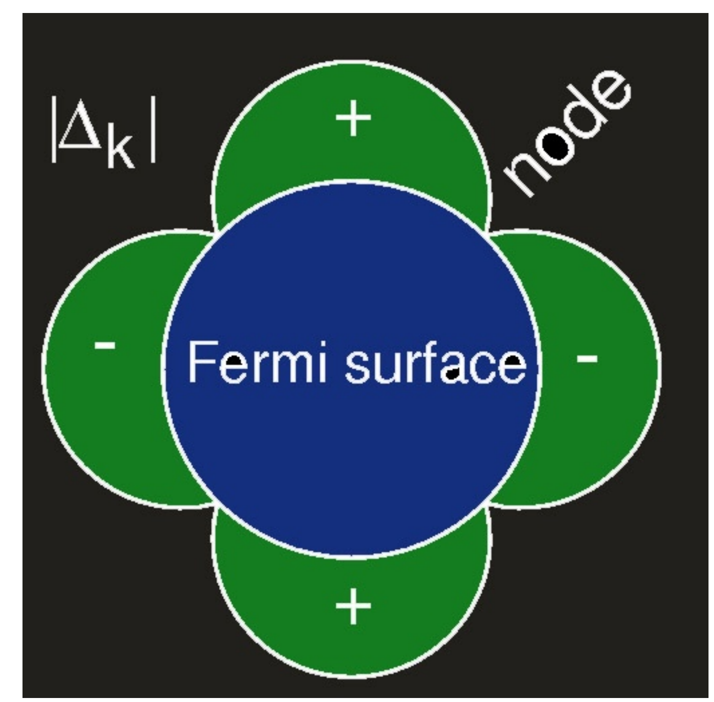
Graphene

## Topological insulators



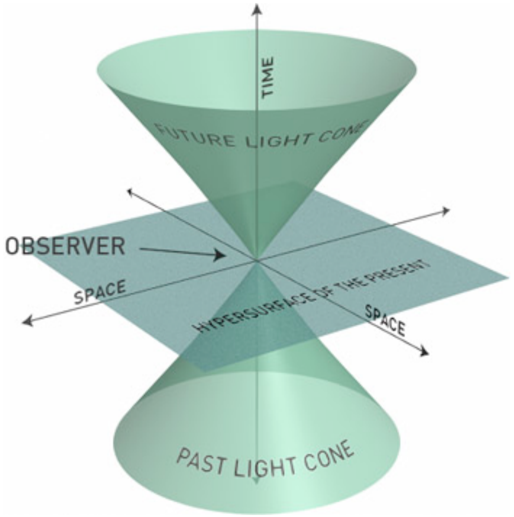

## Nodal superconductors



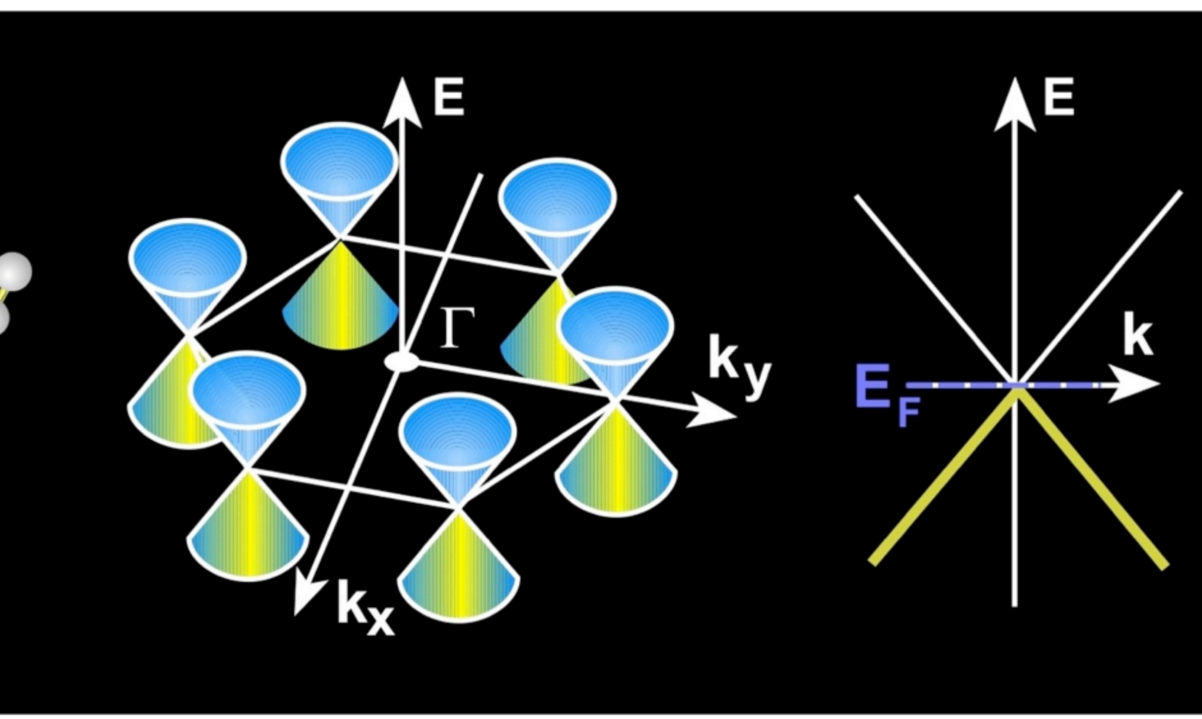



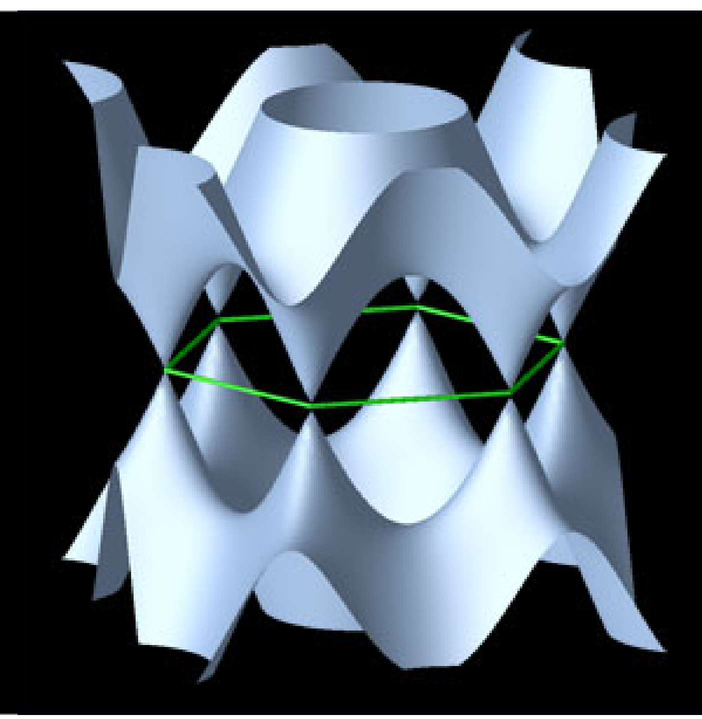

There is a variety of materials that have Dirac fermions as elementary electronic excitations.

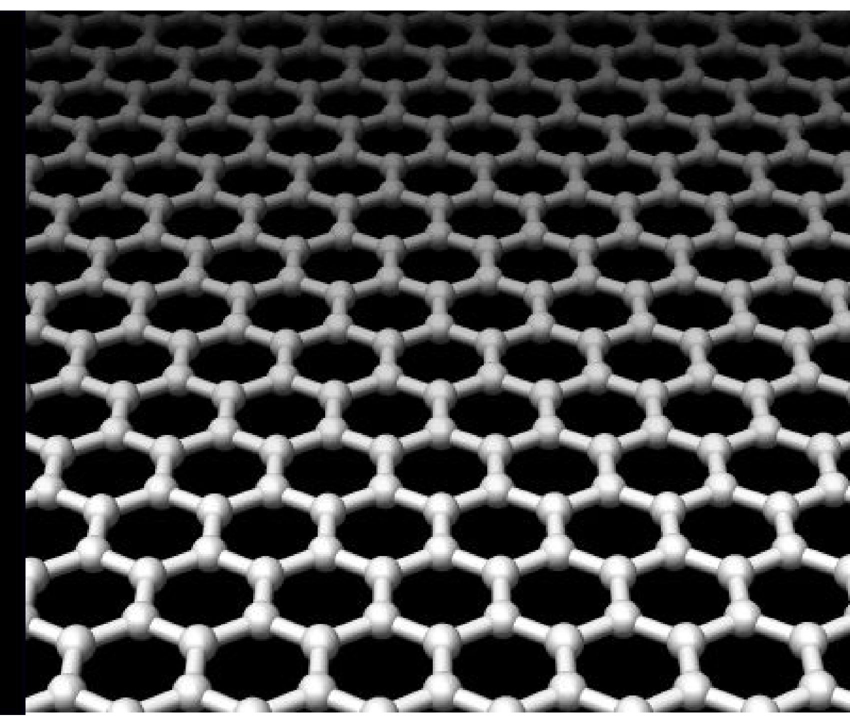
# Dirac fermion physics




"Slow fermions" that behave as Massless neutrinos



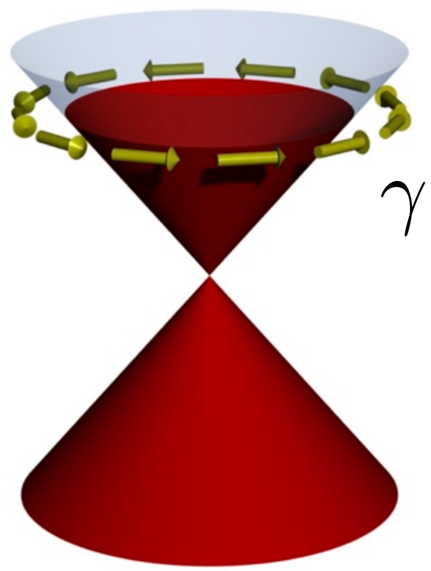





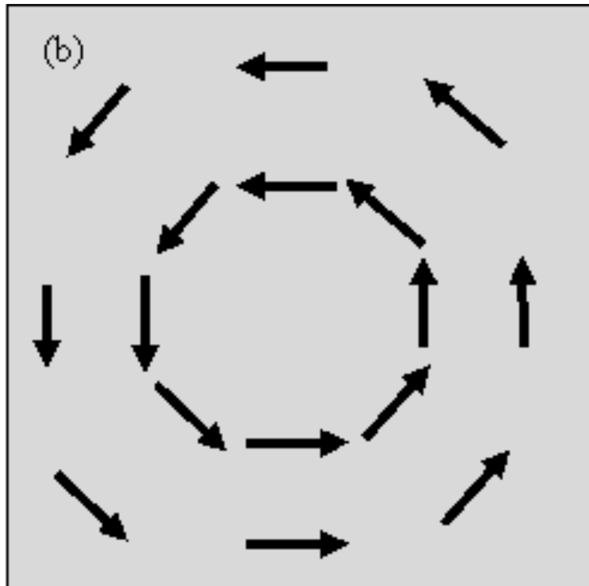
# The crossings in nodal points manifest themselves through band invariants!

Berry phase: $$\gamma = \oint \underbrace{i\langle\Psi|\nabla_{\mathbf{k}}|\Psi\rangle}_{\mathbf{A}} \cdot \mathrm{d}\mathbf{k}$$

Berry connection

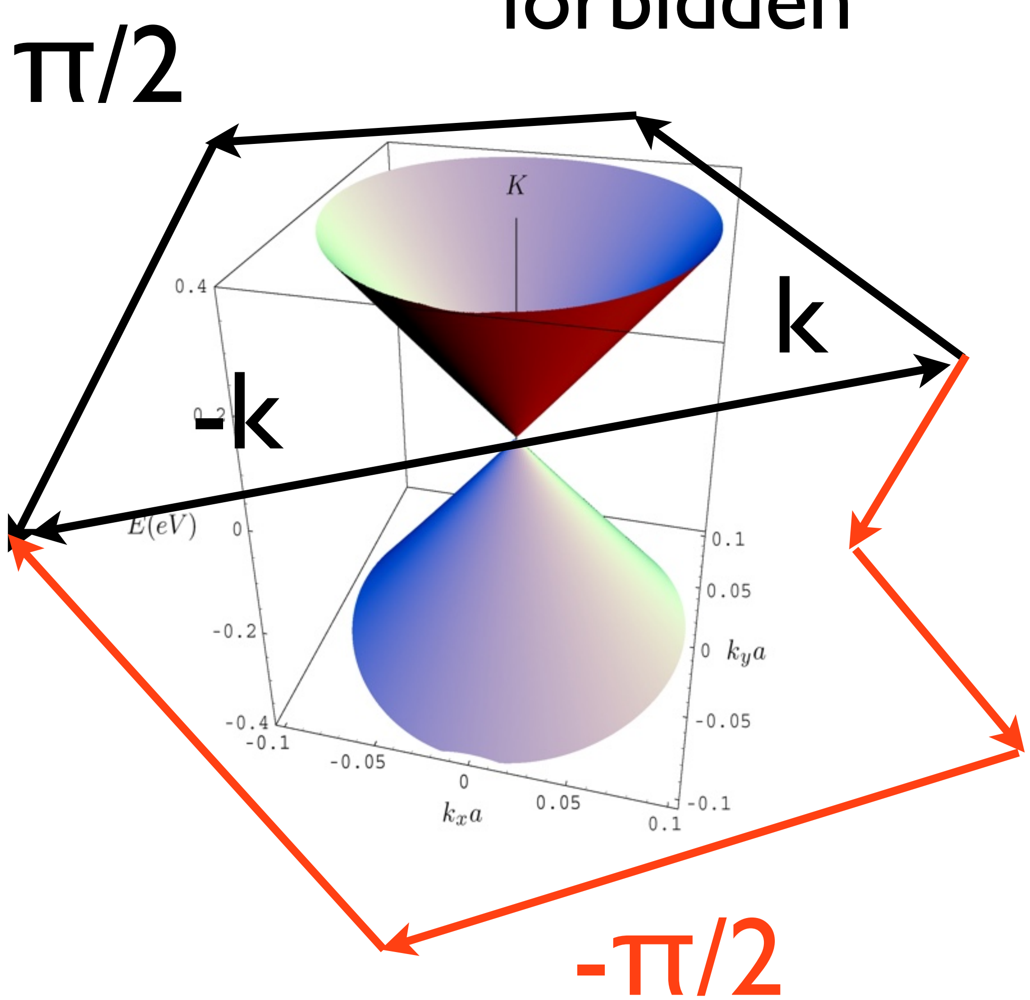



The Berry phase of a nodal crossing with energy spectrum $E(\mathbf{k}) = \pm k^n$, $n \in \mathbb{Z}$ is $\gamma = n\pi$.

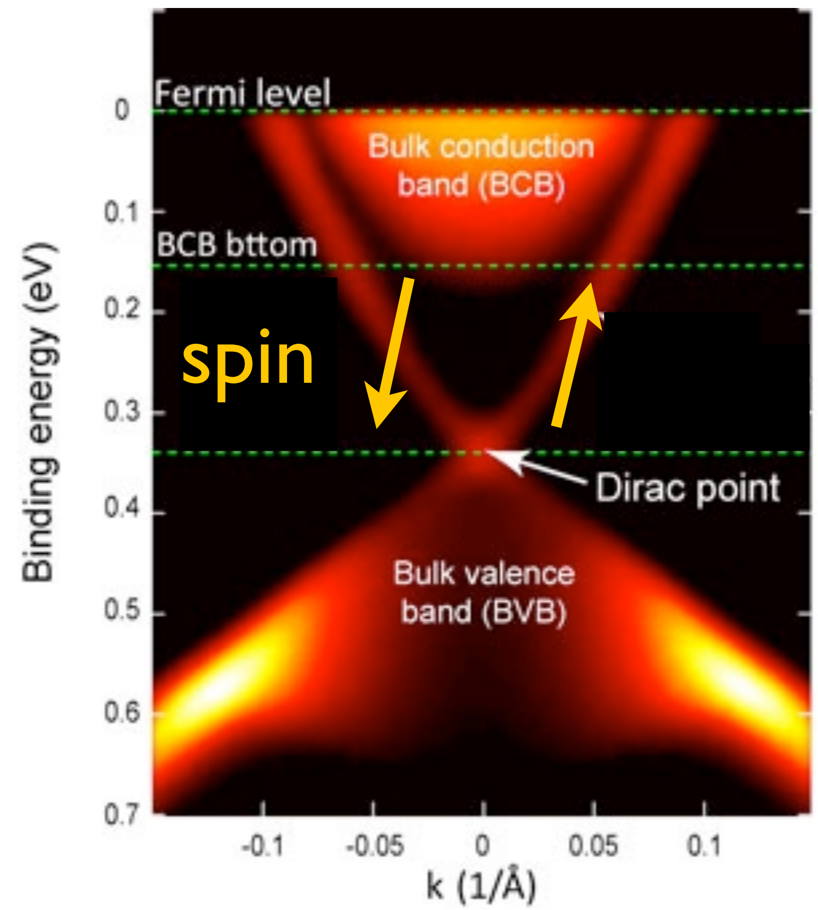


# Dirac materials

Backscattering is topologically forbidden




Topological insulators



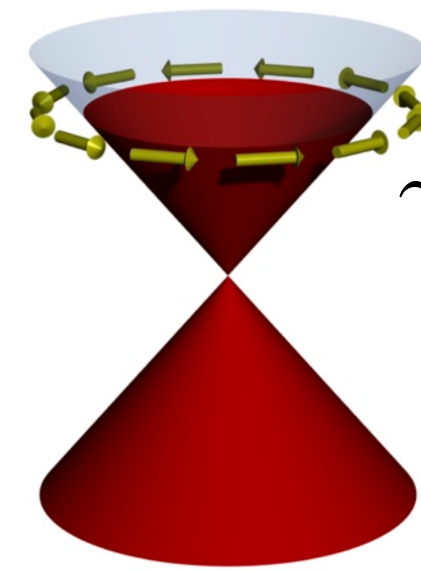

Dirac point is protected
by time reversal symmetry!
(Kramers theorem)

Helical in spin

# The crossings in nodal points manifest themselves through band invariants!

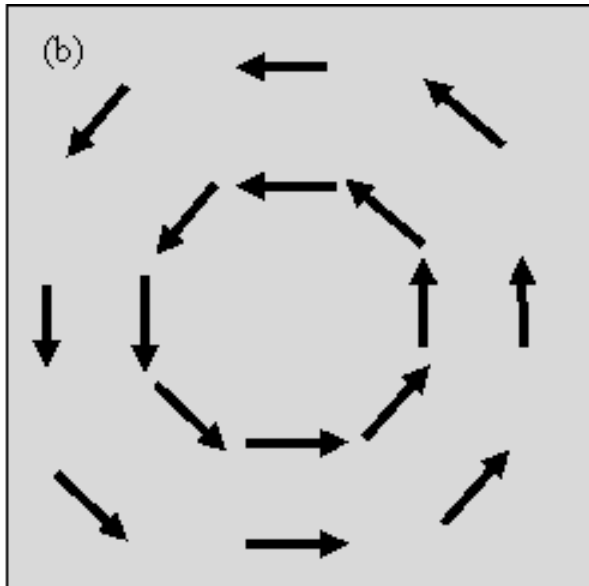
Berry phase: $$\gamma = \oint \underbrace{i\langle\Psi|\nabla_{\mathbf{k}}|\Psi\rangle}_{\mathbf{A}} \cdot d\mathbf{k}$$

Berry connection

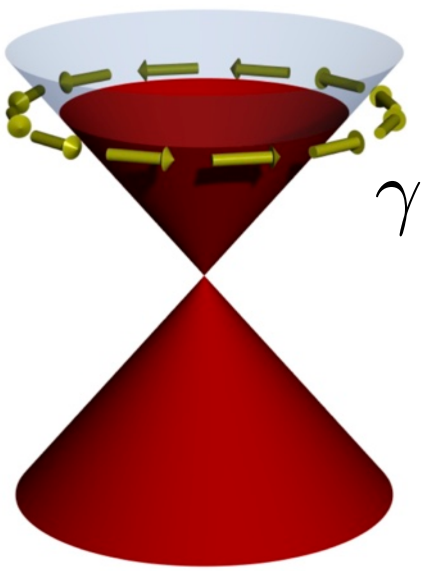


$\gamma = \pi$

The Berry phase of a nodal crossing with energy spectrum $E(\mathbf{k}) = \pm k^n$, $n \in \mathbb{Z}$ is $\gamma = n\pi$.



# The crossings in nodal points manifest themselves through band invariants!




Berry phase: $$\gamma = \oint \underbrace{i\langle\Psi|\nabla_{\mathbf{k}}|\Psi\rangle}_{\mathbf{A}} \cdot d\mathbf{k}$$

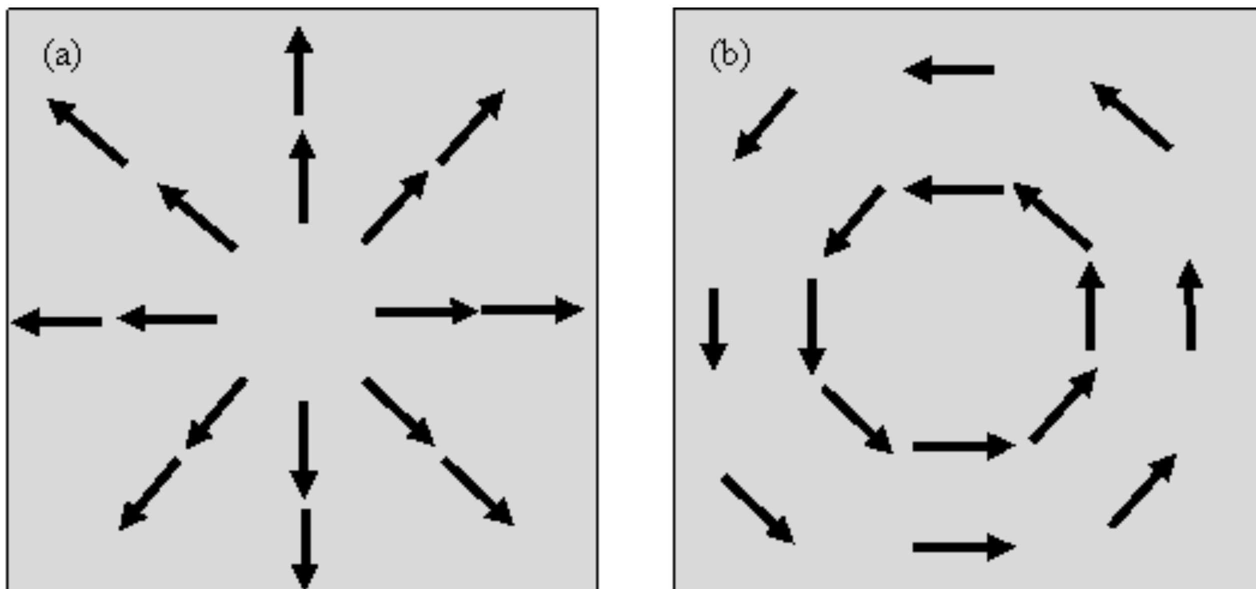
Berry connection

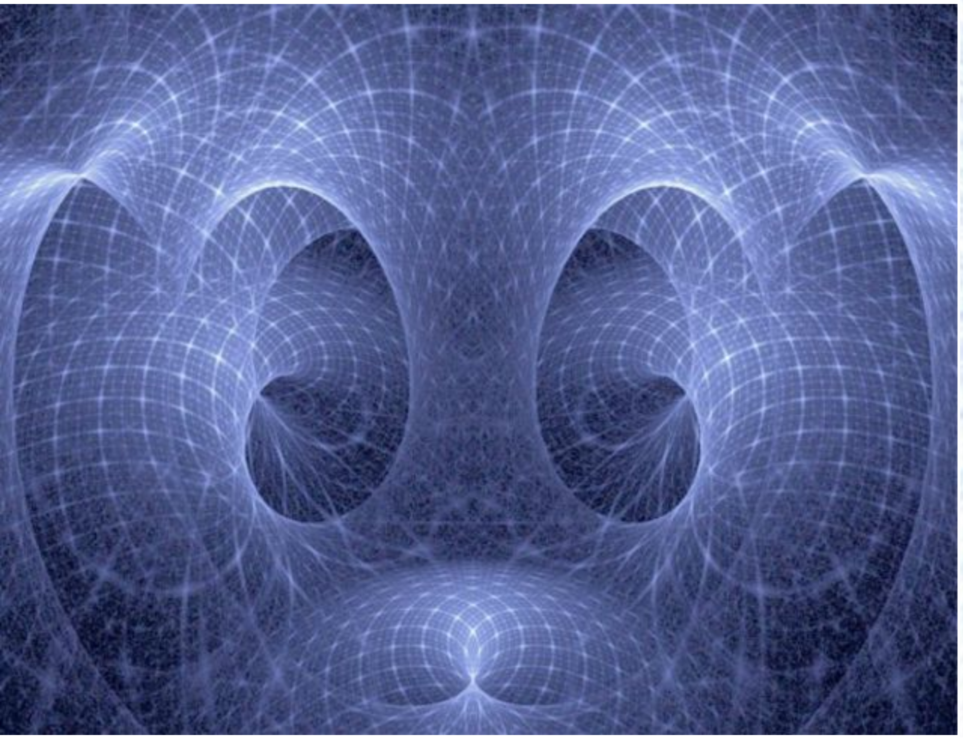
Chern number: $$\nu = \int\int d\mathbf{S} \cdot \underbrace{\nabla_{\mathbf{k}} \times i\langle\Psi|\nabla_{\mathbf{k}}|\Psi\rangle}_{\vec{\Omega}}$$

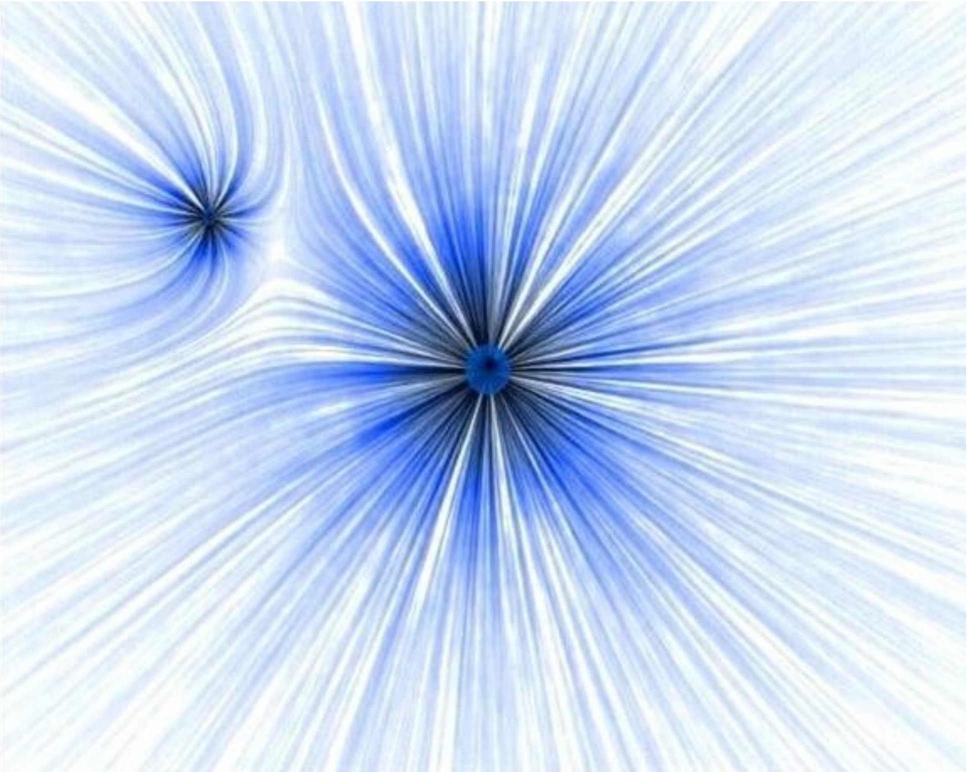
Berry curvature

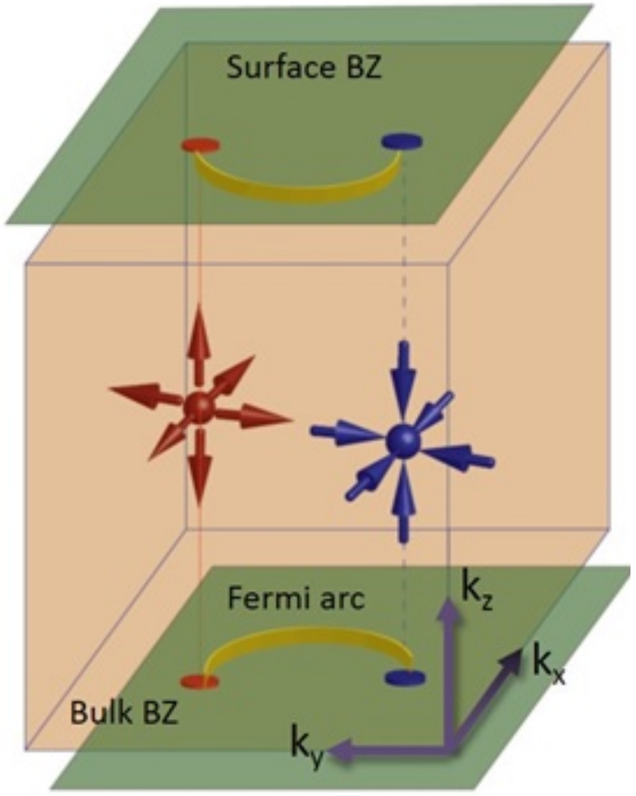
The Berry curvature is the analog of a magnetic field.

In 3D, the Chern number is the analog of the flux produced by a magnetic monopole!

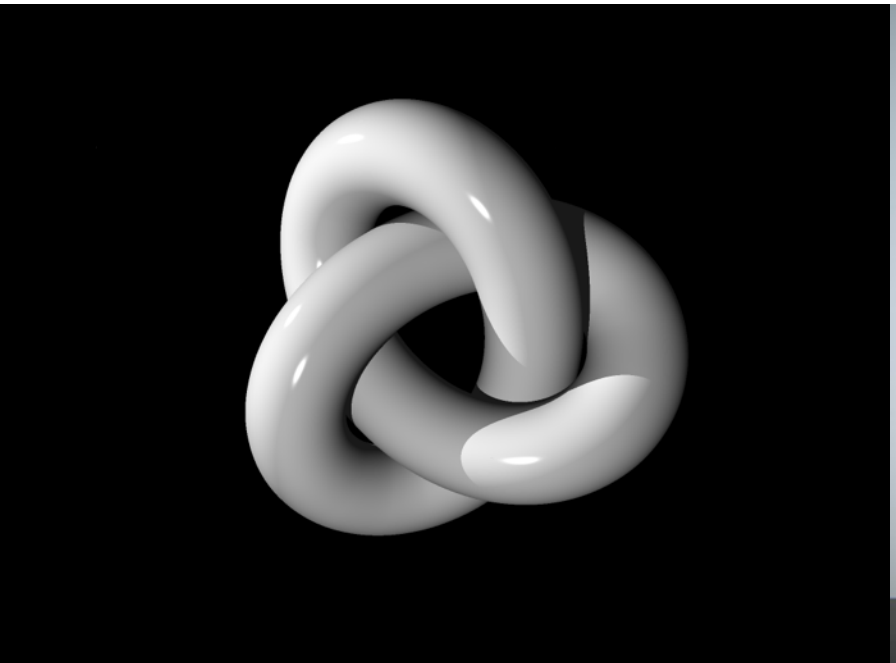


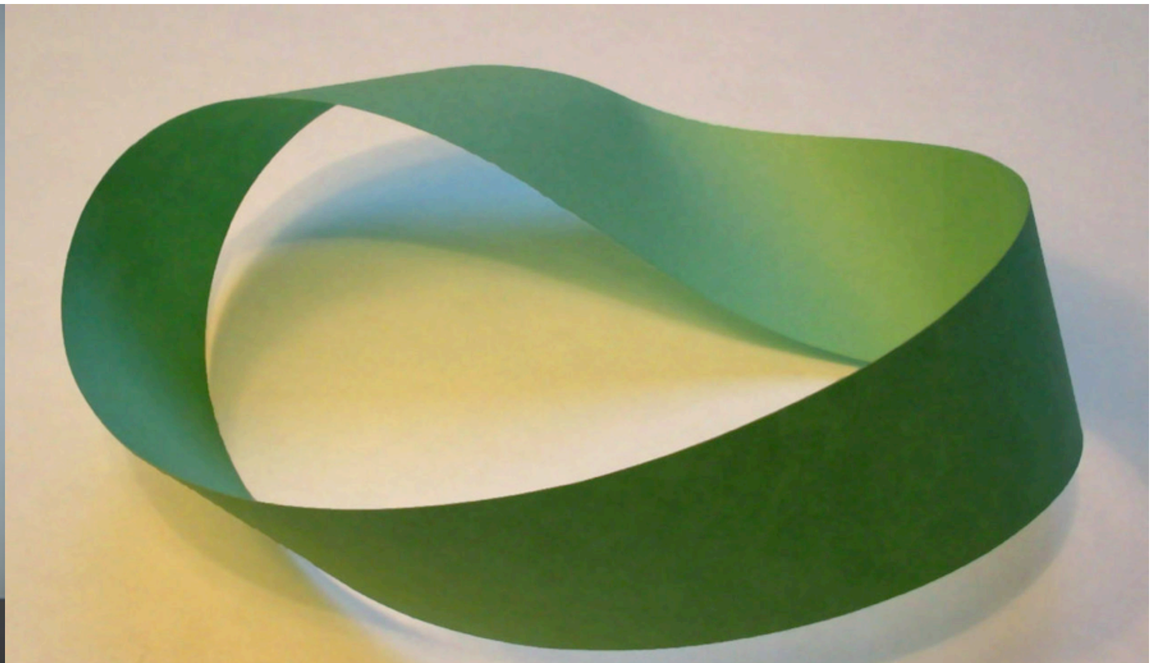


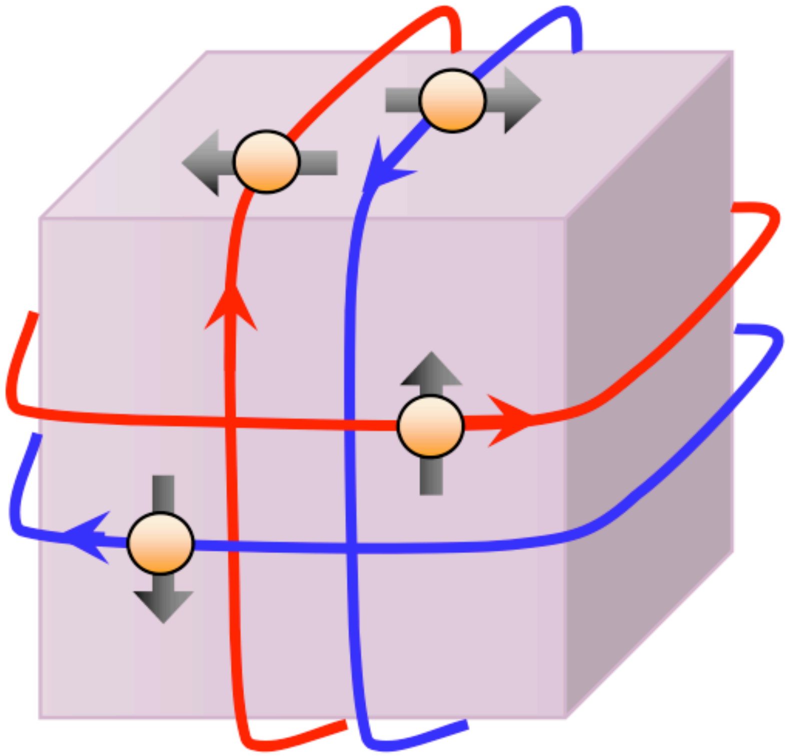


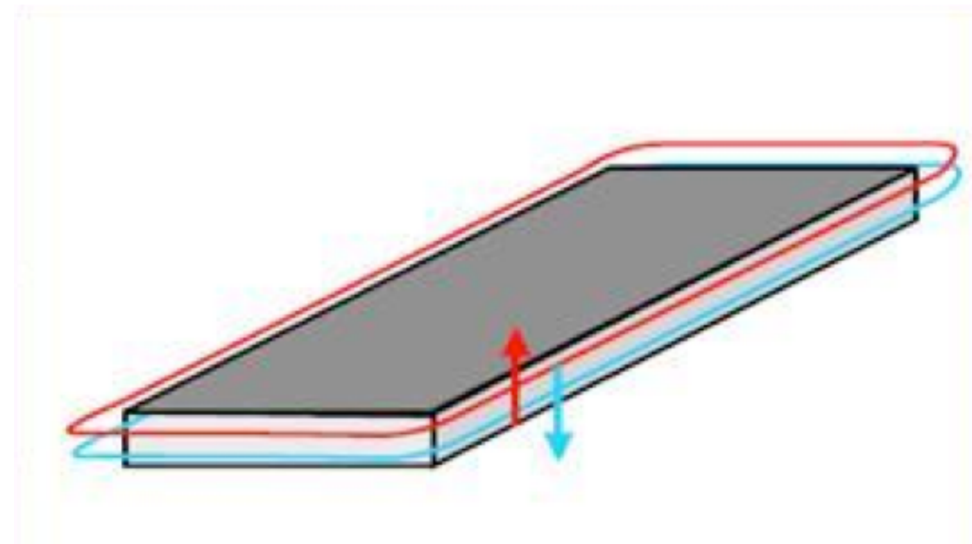



In 3D materials, those “magnetic monopoles” are connected to each other by Dirac strings!

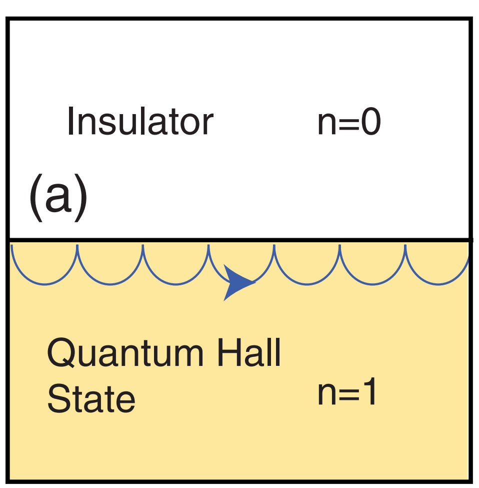


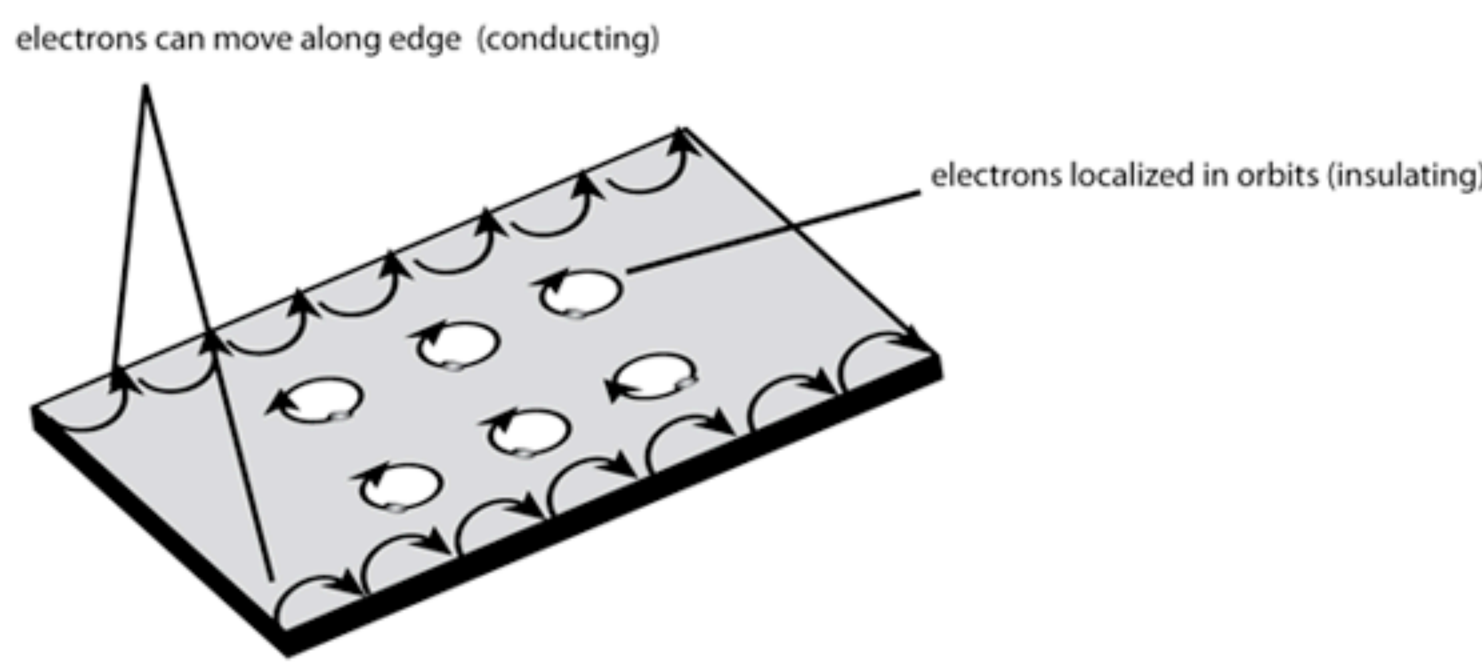




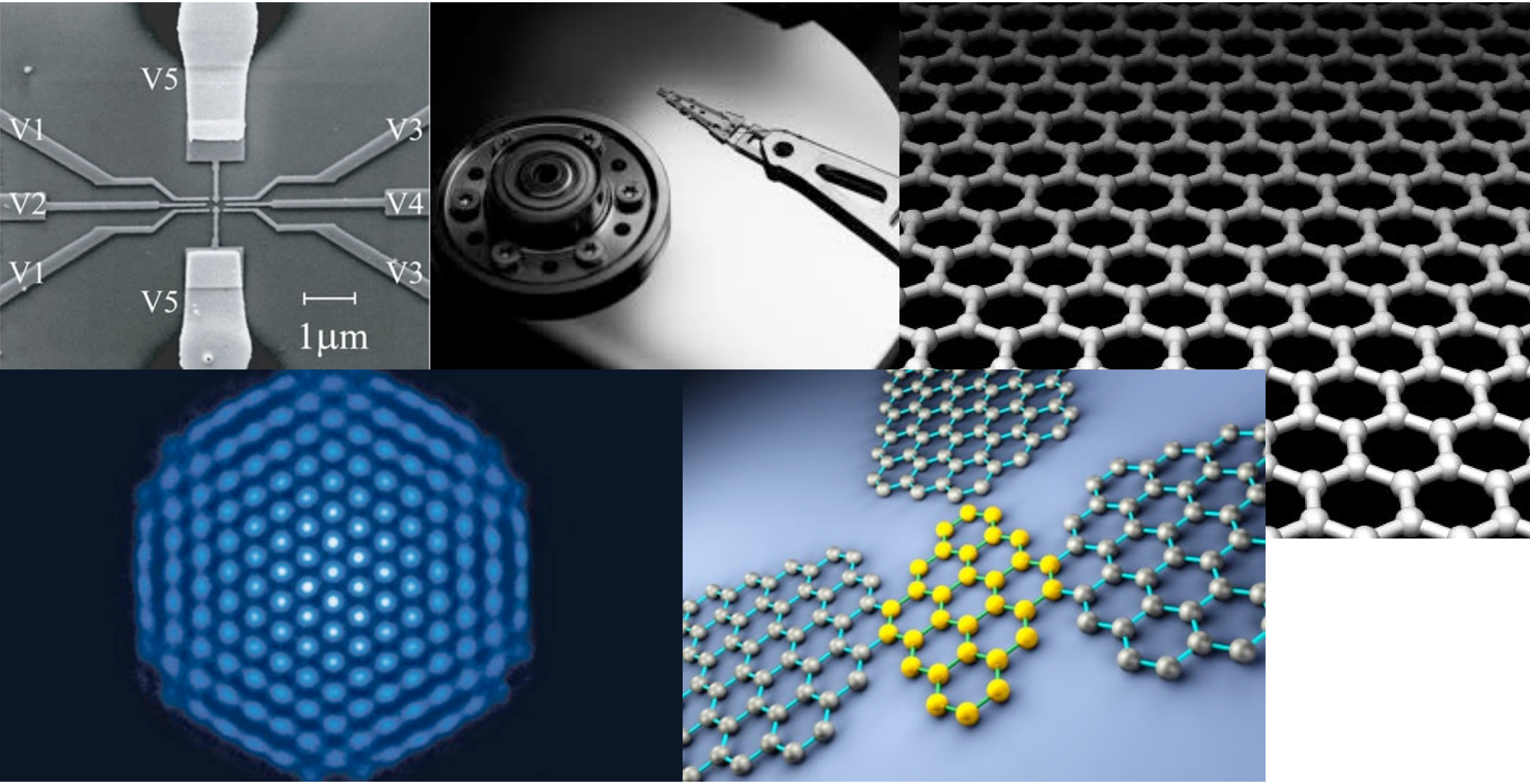


All topological materials are insulators in bulk and metallic at the surface!



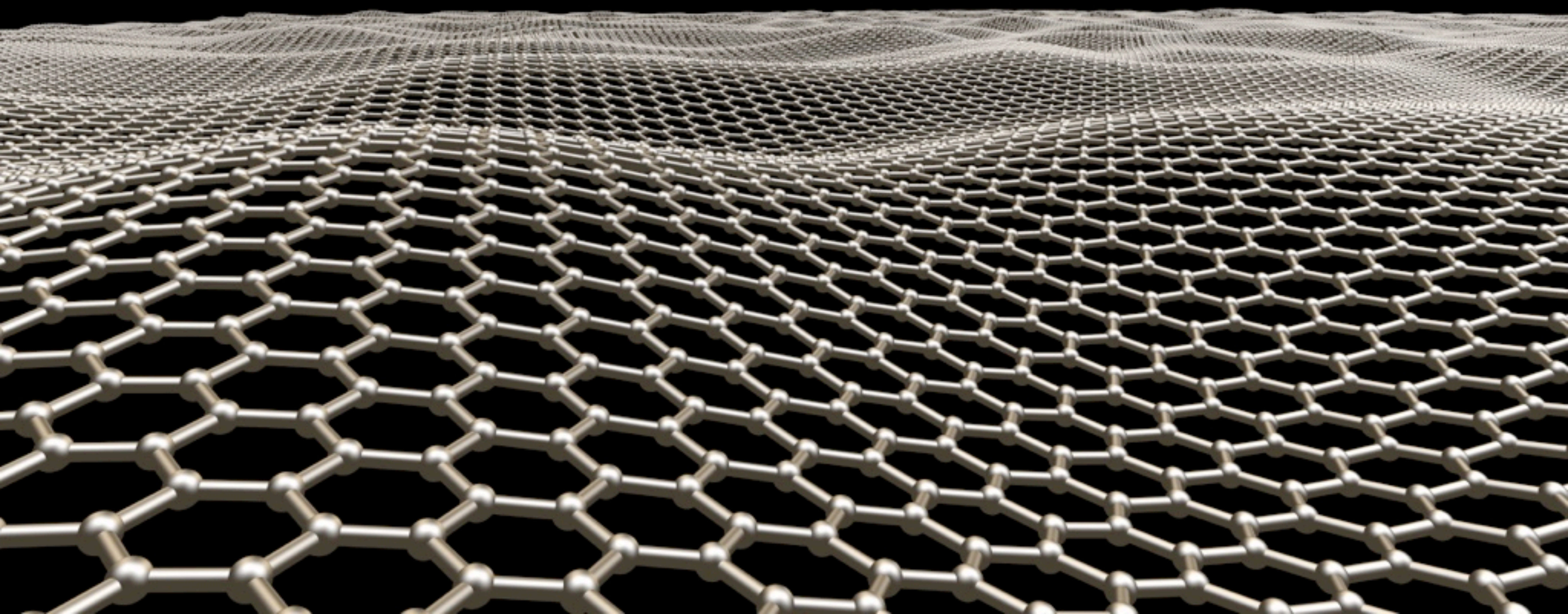



# Nano science

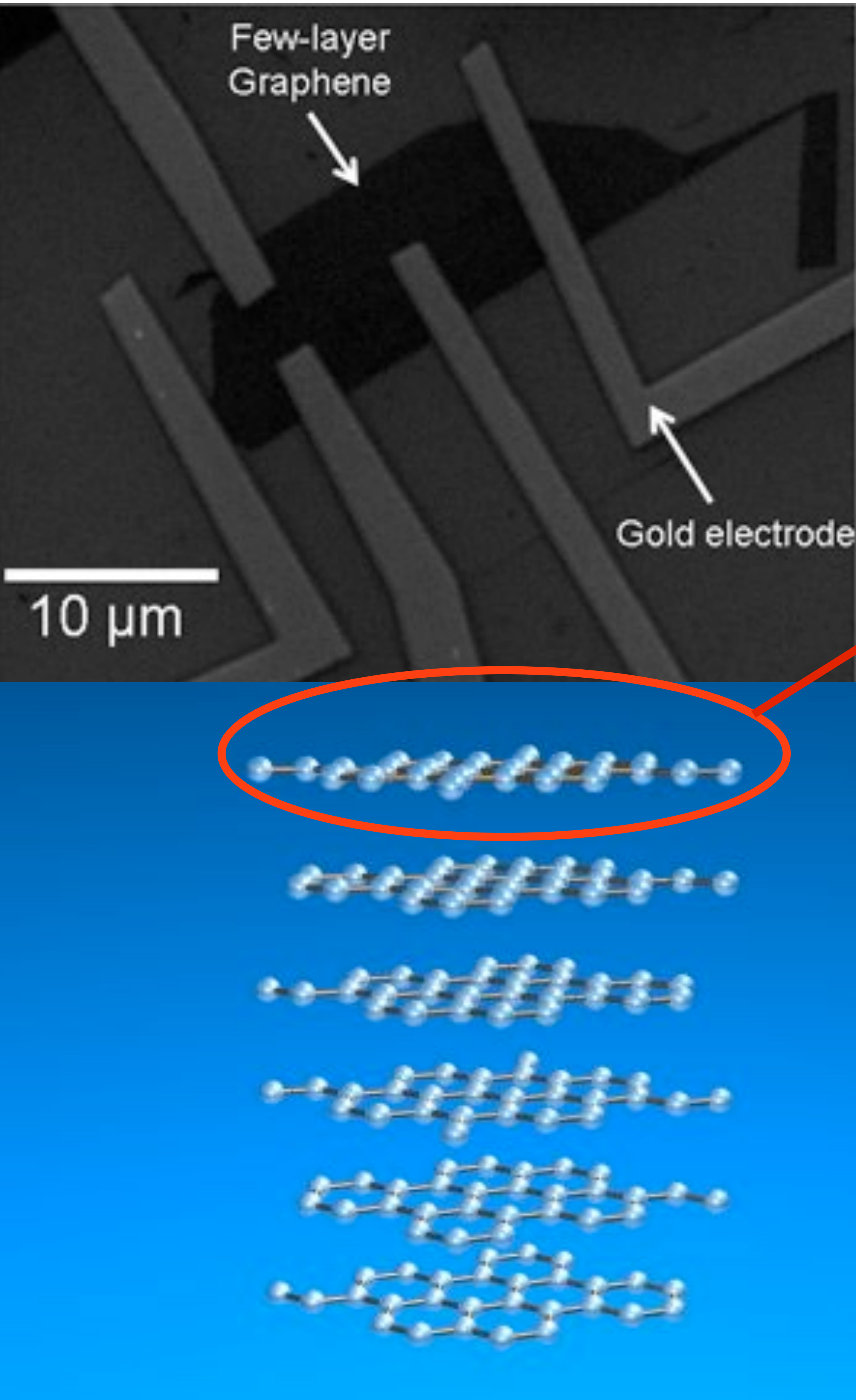



Novel materials can be tailored at mesoscopic sizes for new purposes!

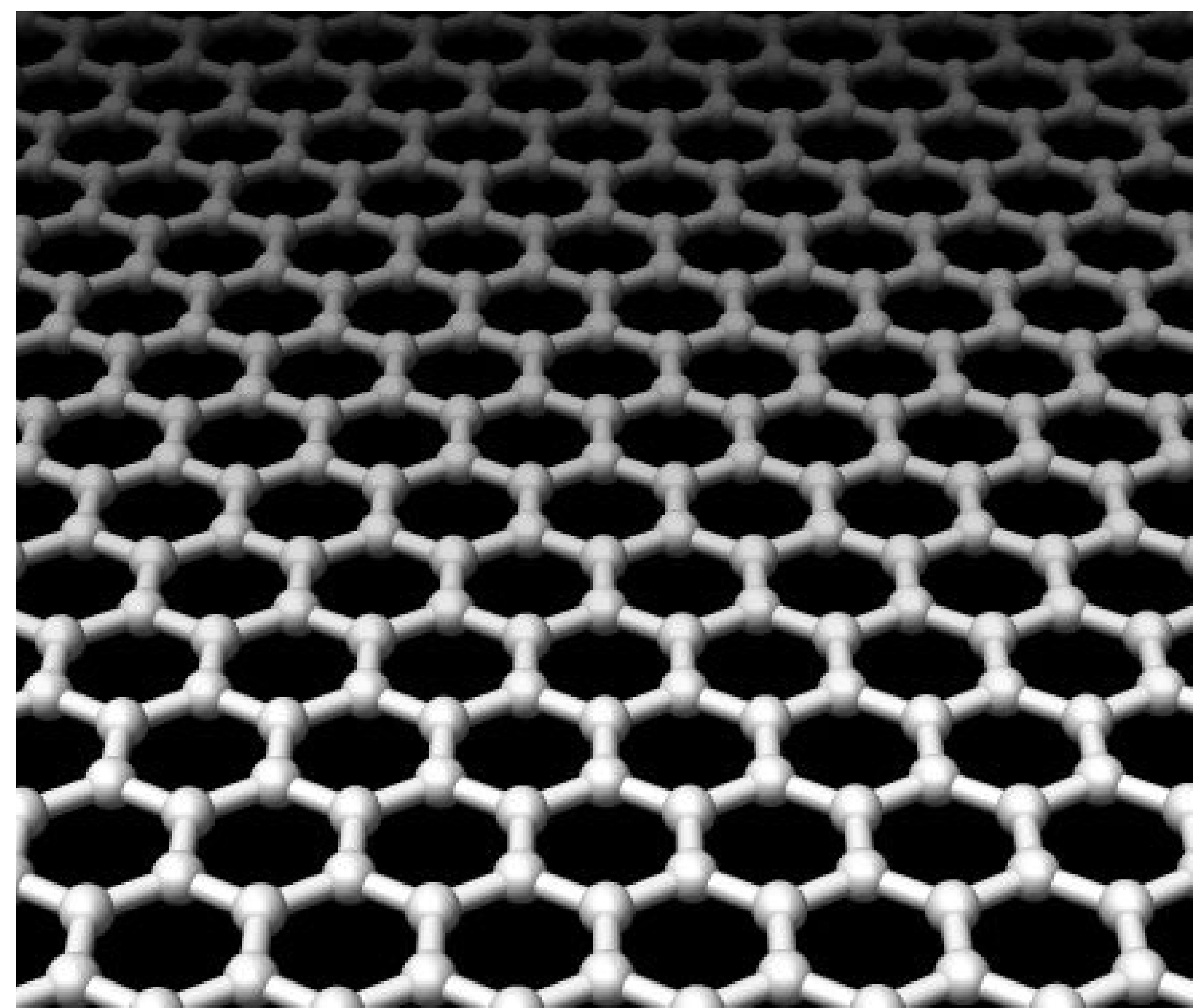
# Graphene



# The thinnest material in the universe




1 atom thick sheet of graphite!

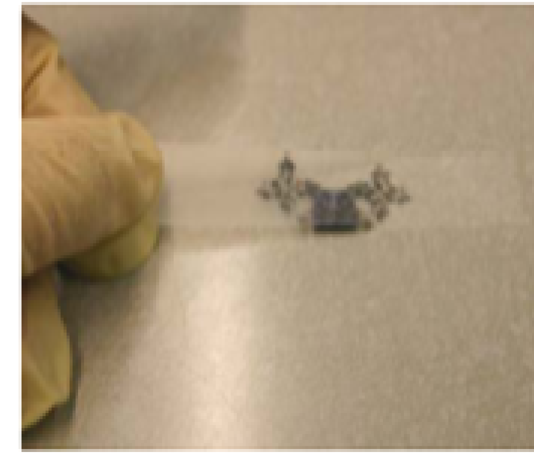


666 22 OCTOBER 2004 VOL 306 SCIENCE

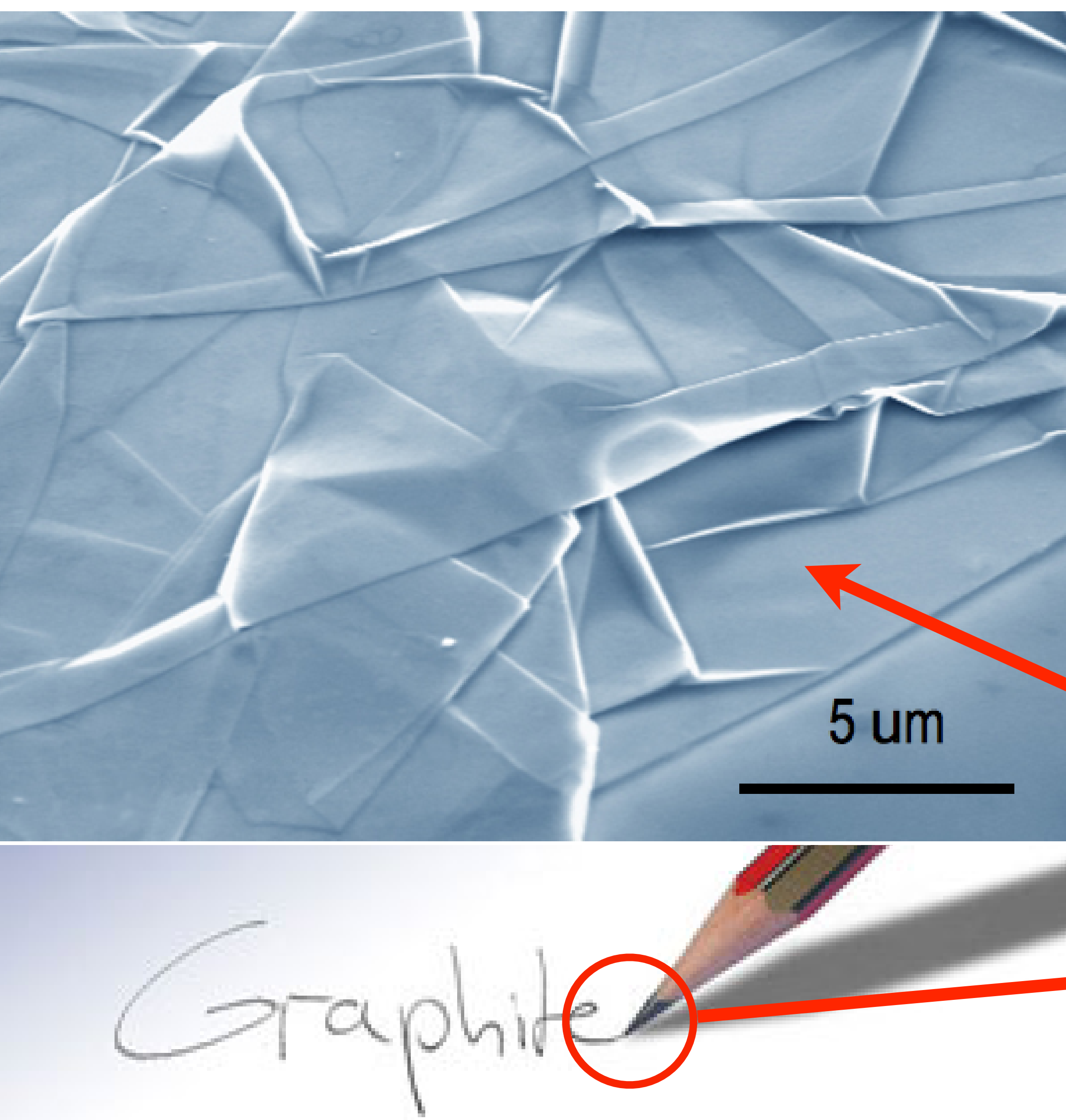
# Electric Field Effect in Atomically Thin Carbon Films

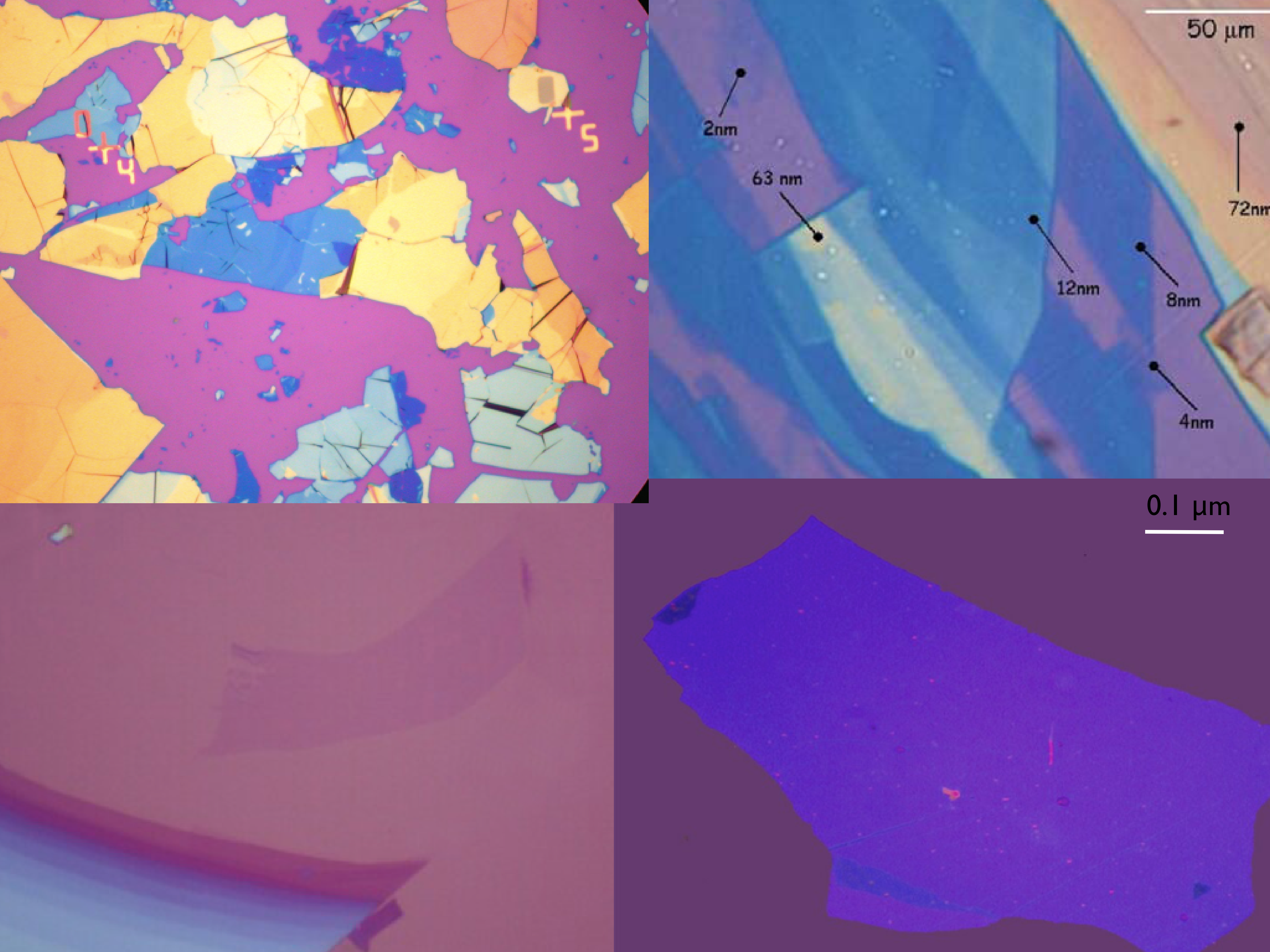
K. S. Novoselov,[1] A. K. Geim,[1*] S. V. Morozov,[2] D. Jiang,[1]
Y. Zhang,[1] S. V. Dubonos,[2] I. V. Grigorieva,[1] A. A. Firsov[2]

We describe monocrystalline graphitic films, which are a few atoms thick but are nonetheless stable under ambient conditions, metallic, and of remarkably high



Pealing graphite with adhesive tape!





50 µm
2nm
63 nm
12nm
8nm
4nm
0.1 µm

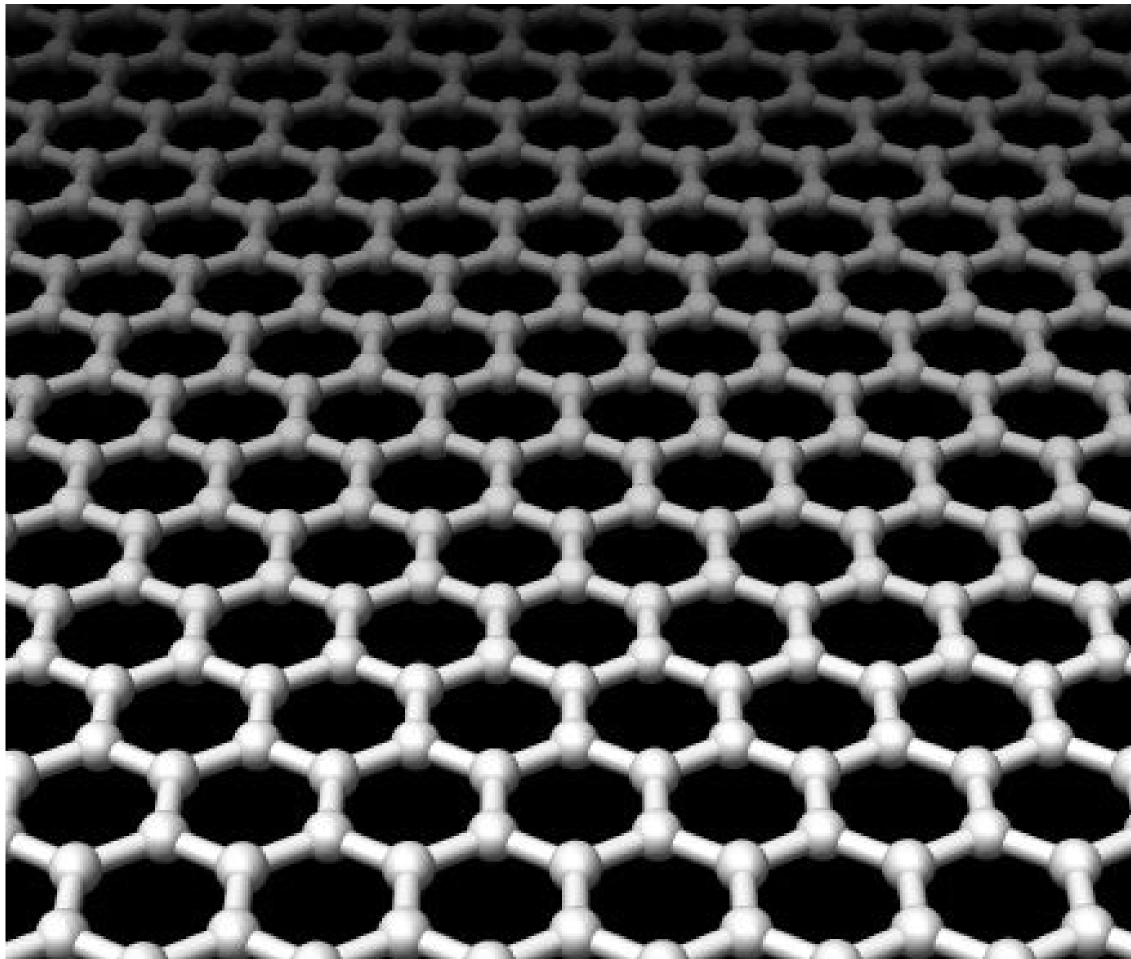
# The Nobel Prize in Physics 2010
## Andre Geim, Konstantin Novoselov

**Andre Geim**
University of Manchester, UK

and

**Konstantin Novoselov**
University of Manchester, UK

*"for groundbreaking experiments regarding the two-dimensional material graphene"*



Eur. J. Phys. 18 (1997) 307–313. Printed in the UK PII: S0143-0807(97)84689-2

# Of flying frogs and levitrons

M V Berry† and A K Geim‡

**Figure 4(*b*).** Frog levitated in the stable region.

Eur. J. Phys. 18 (1997) 307–313. Printed in the UK

PII: S0143-0807(97)84689-2

# Of flying frogs and levitrons

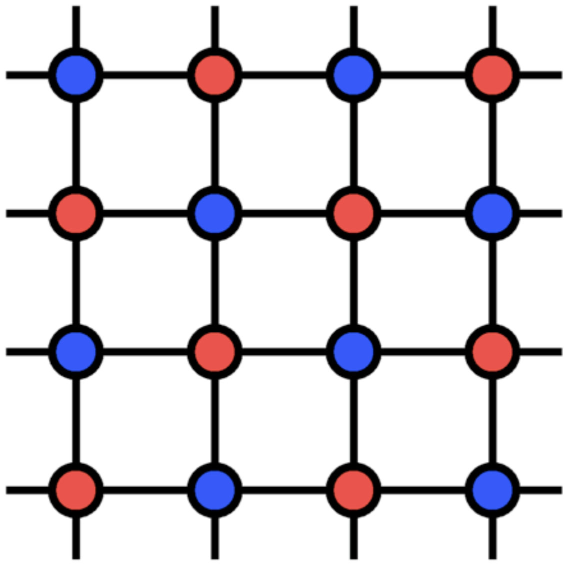
M V Berry† and A K Geim‡

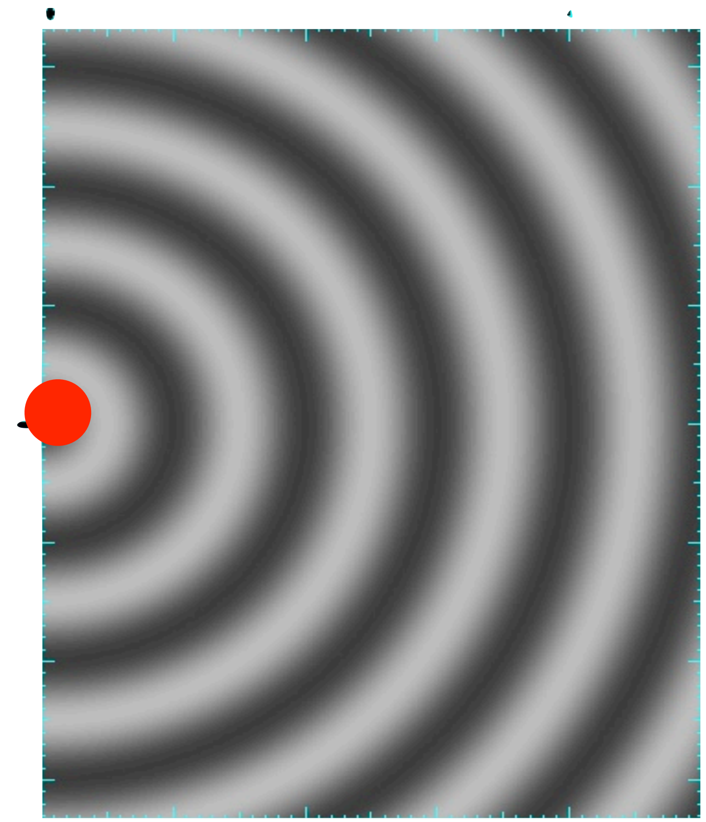
2000 IgNobel prize in physics

For achievements that first make people laugh and then make people think

**Figure 4(*b*).** Frog levitated in the stable region.

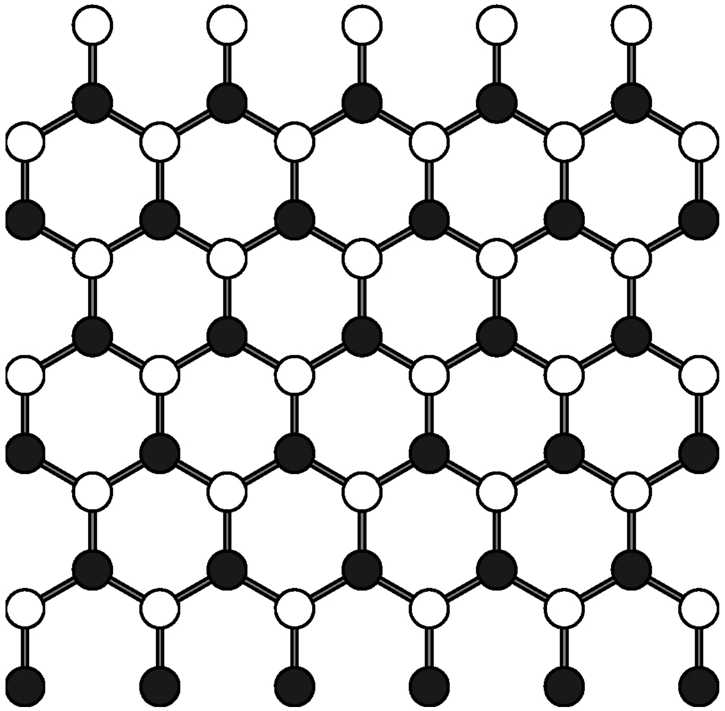
# Square lattice



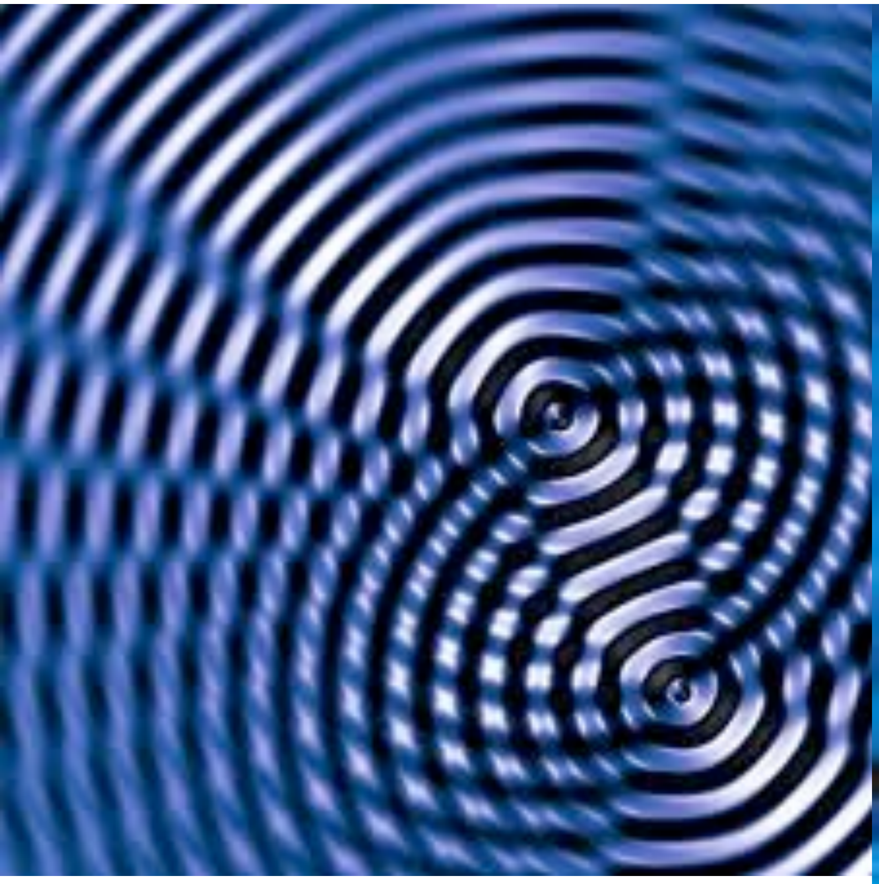


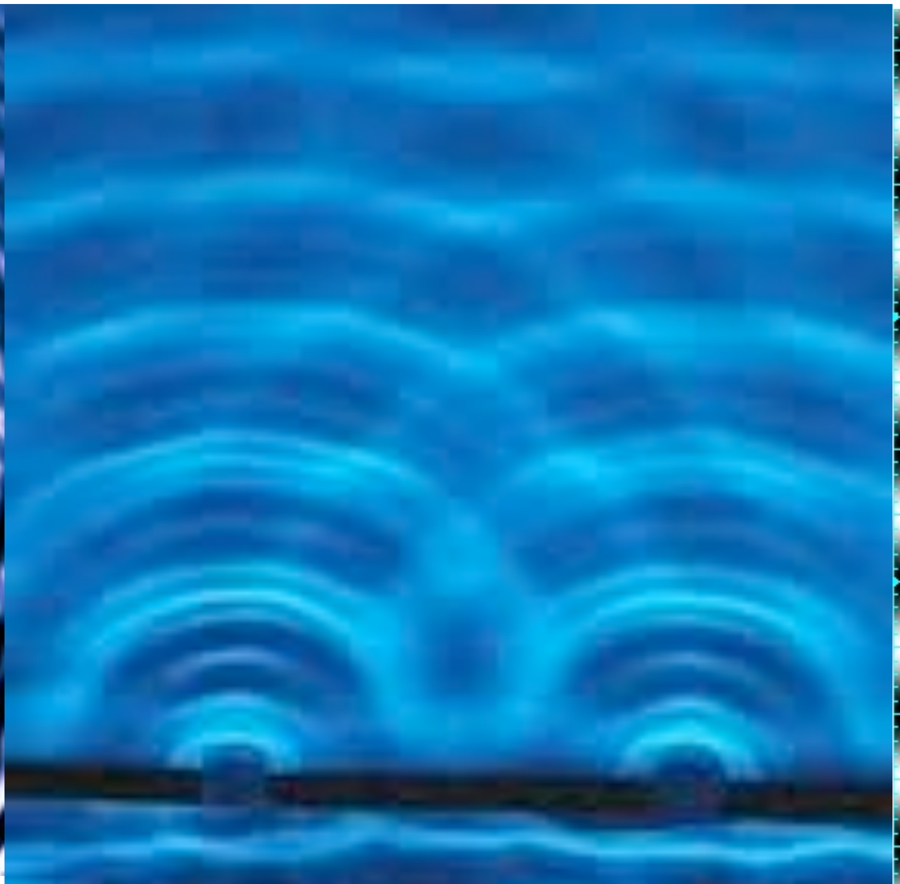
# Particle-wave duality

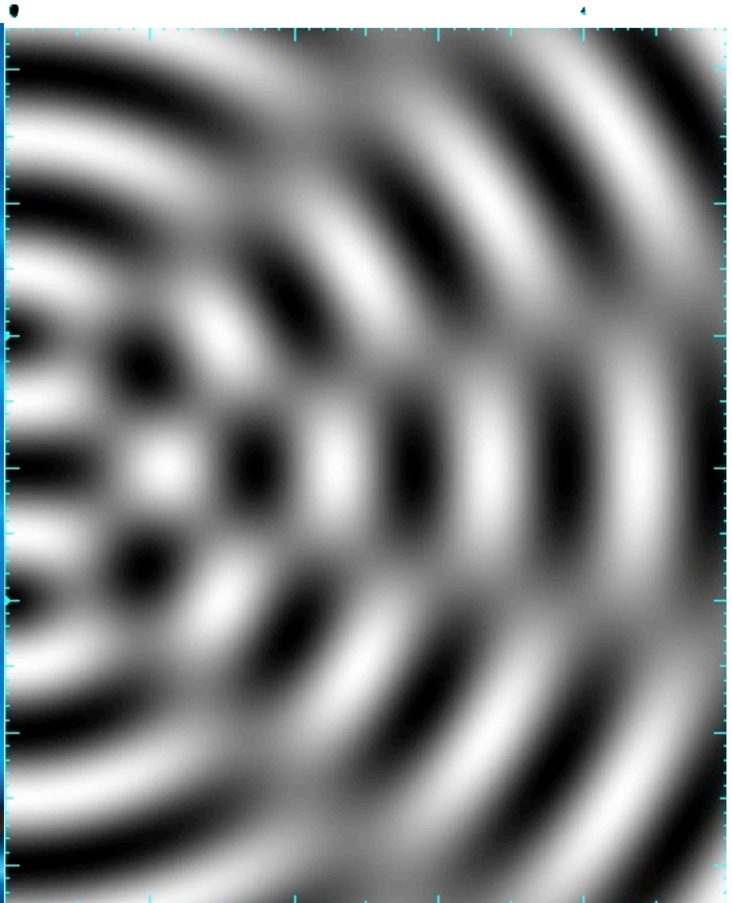
# Honeycomb lattice (chicken wire)



Interference!



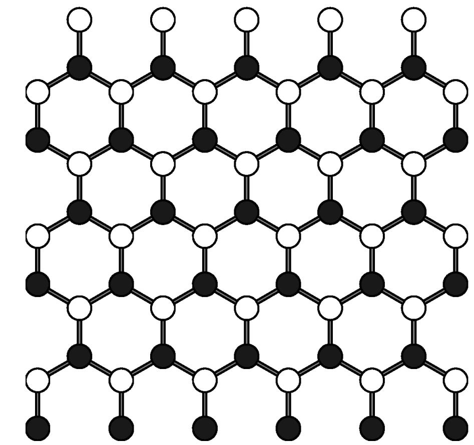




$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+V(\mathbf{r})\Psi(\mathbf{r},t)$$

+

Honeycomb lattice



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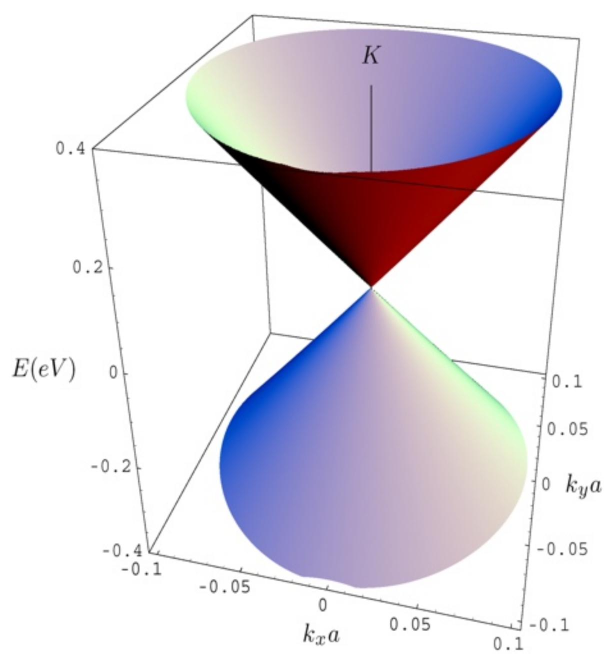
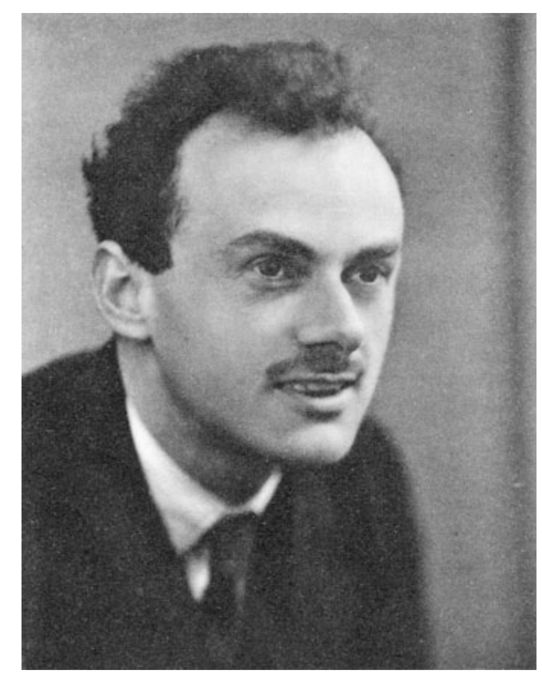



$$E(p) = \pm v\, p$$

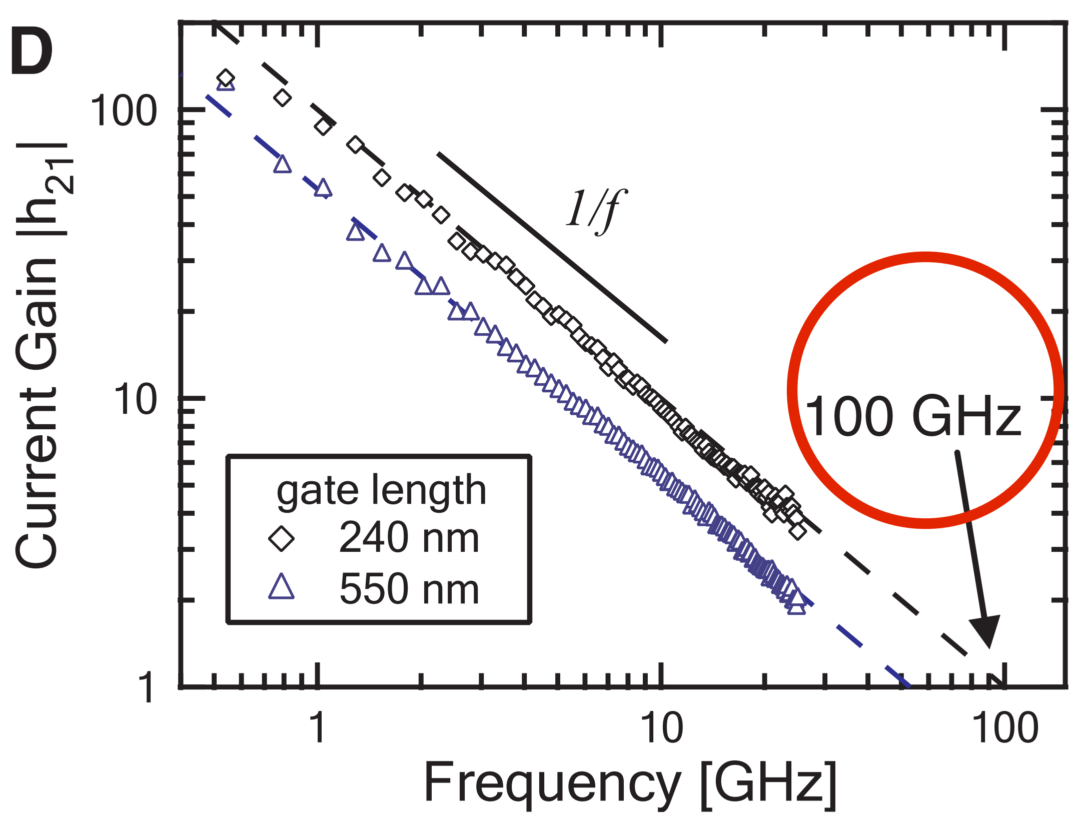


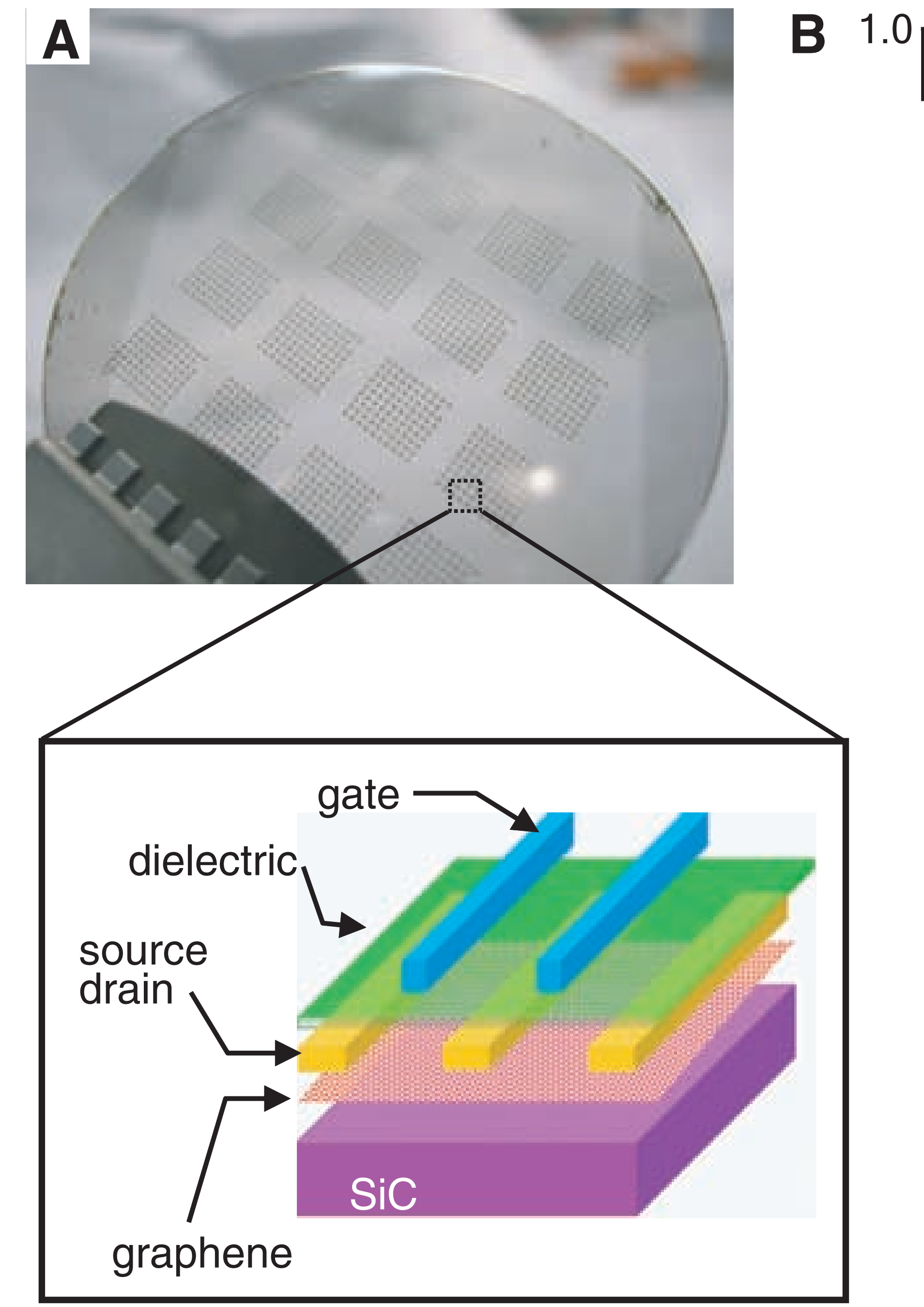
Massless Dirac fermions!

# Very high electronic mobility at room temperature

## 100-GHz Transistors from Wafer-Scale Epitaxial Graphene

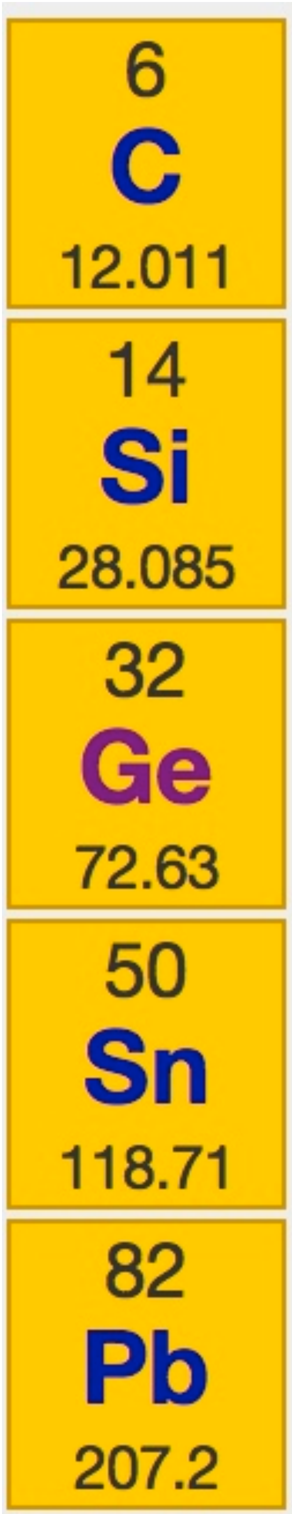
Y.-M. Lin,* C. Dimitrakopoulos, K. A. Jenkins, D. B. Farmer, H.-Y. Chiu, A. Grill, Ph. Avouris*



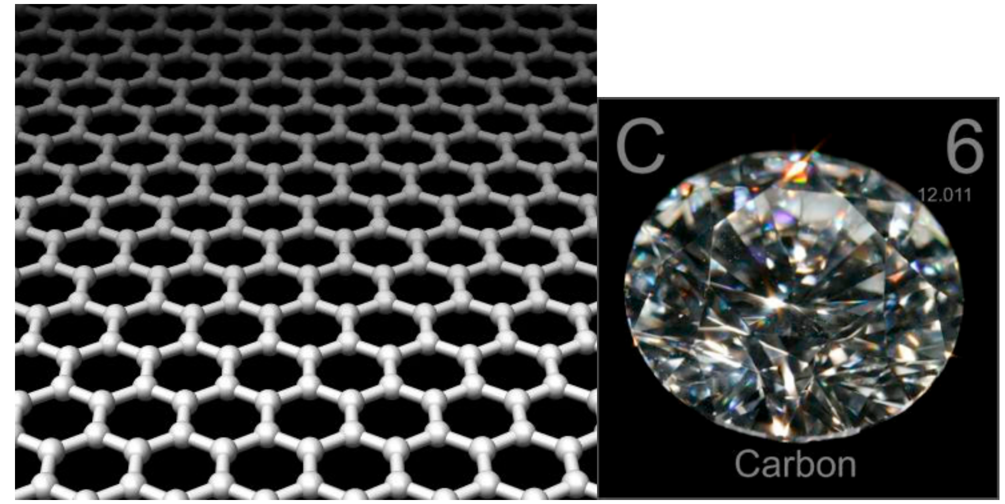




Ultra-fast transistors!

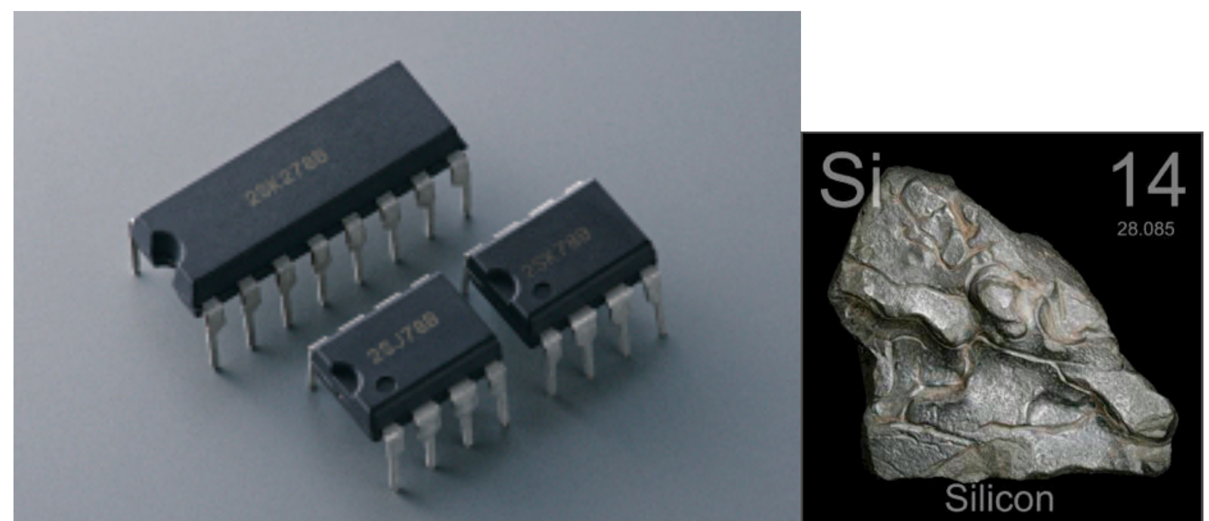
# Periodic table




Carbon based transistors?




Silicon industry



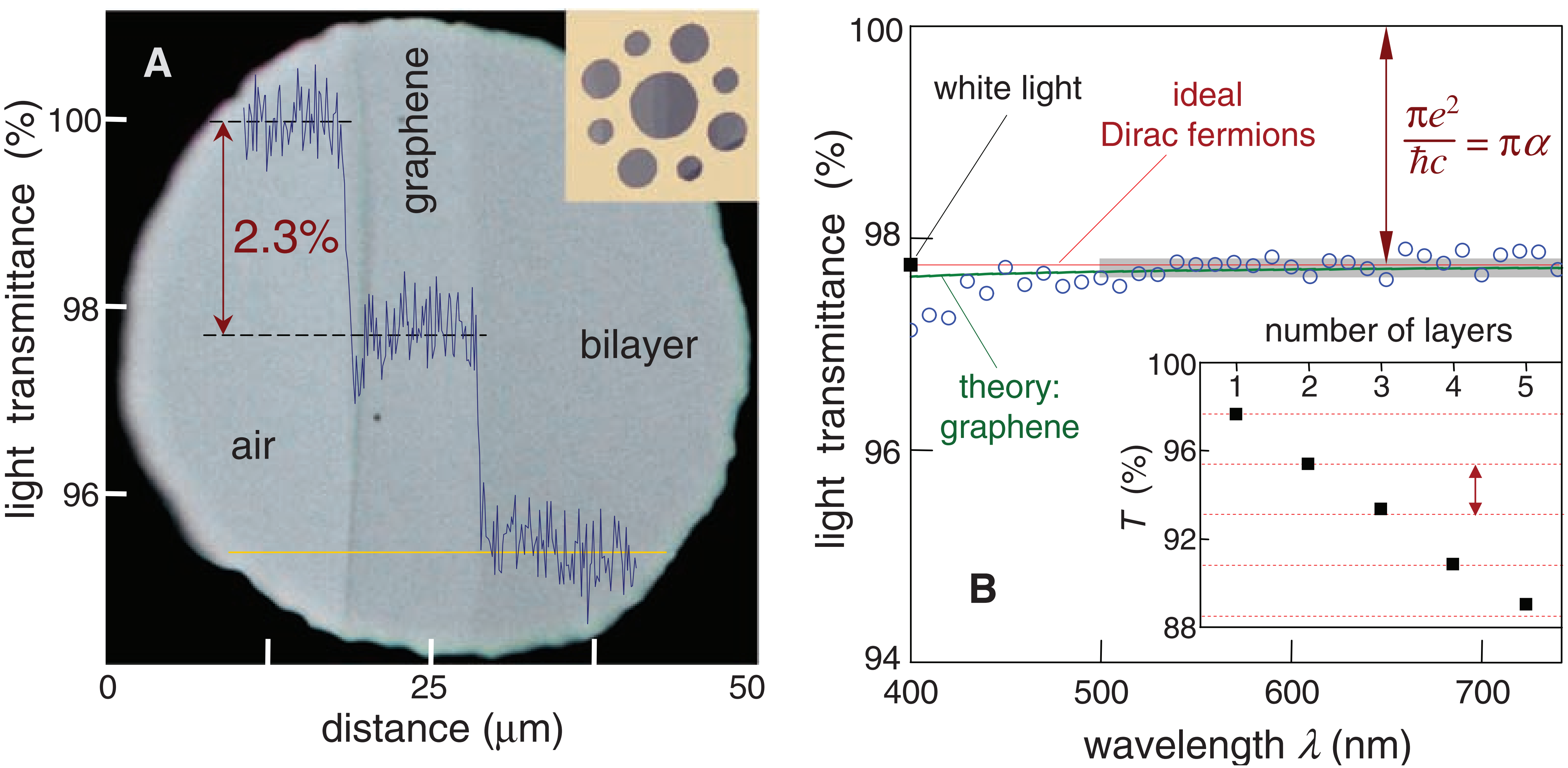

Ge transistor (1947)


Time

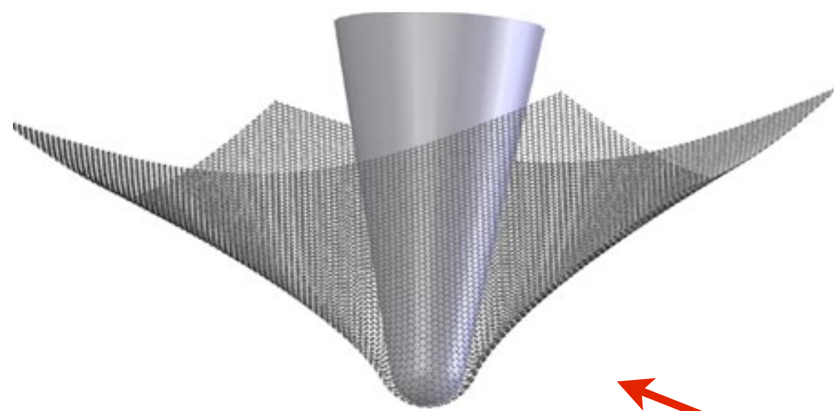
# Fine Structure Constant Defines Visual Transparency of Graphene

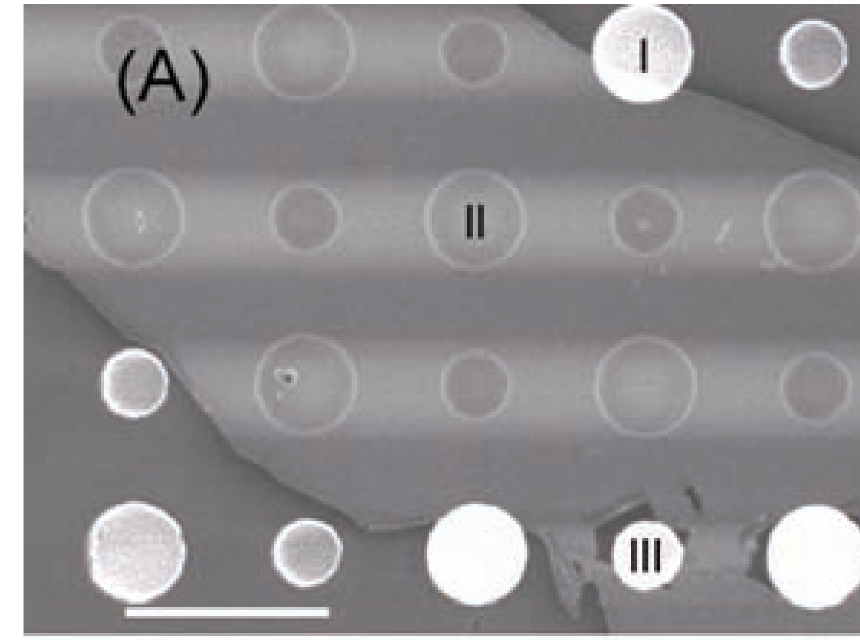
Very transparent

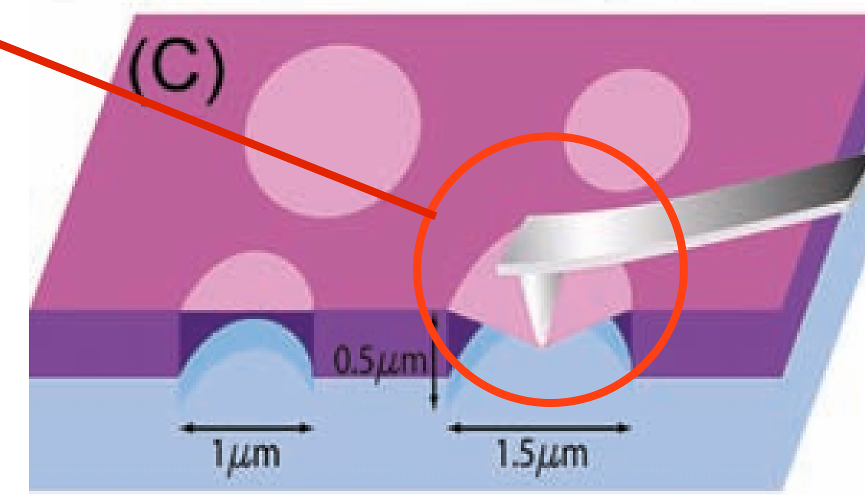
R. R. Nair,[1] P. Blake,[1] A. N. Grigorenko,[1] K. S. Novoselov,[1] T. J. Booth,[1] T. Stauber,[2] N. M. R. Peres,[2] A. K. Geim[1]*

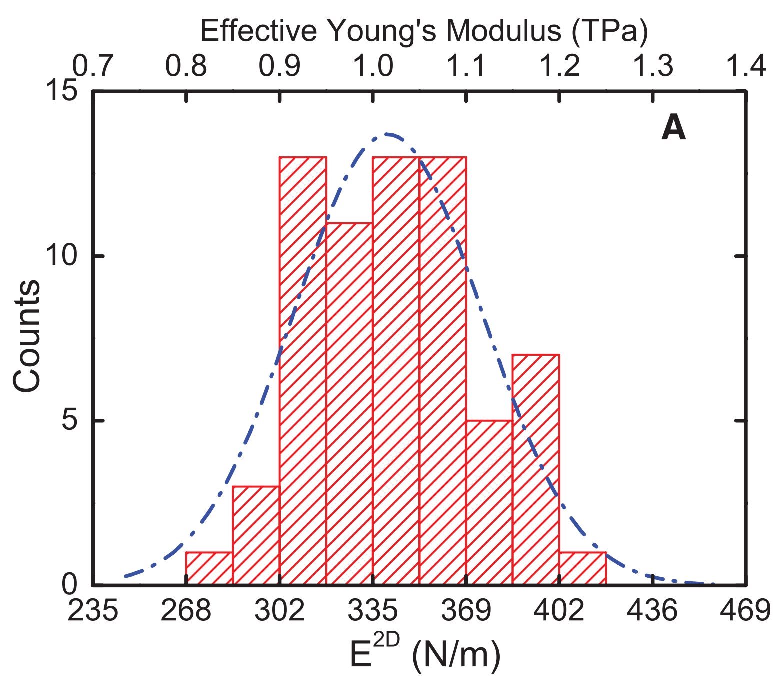


# The strongest known material

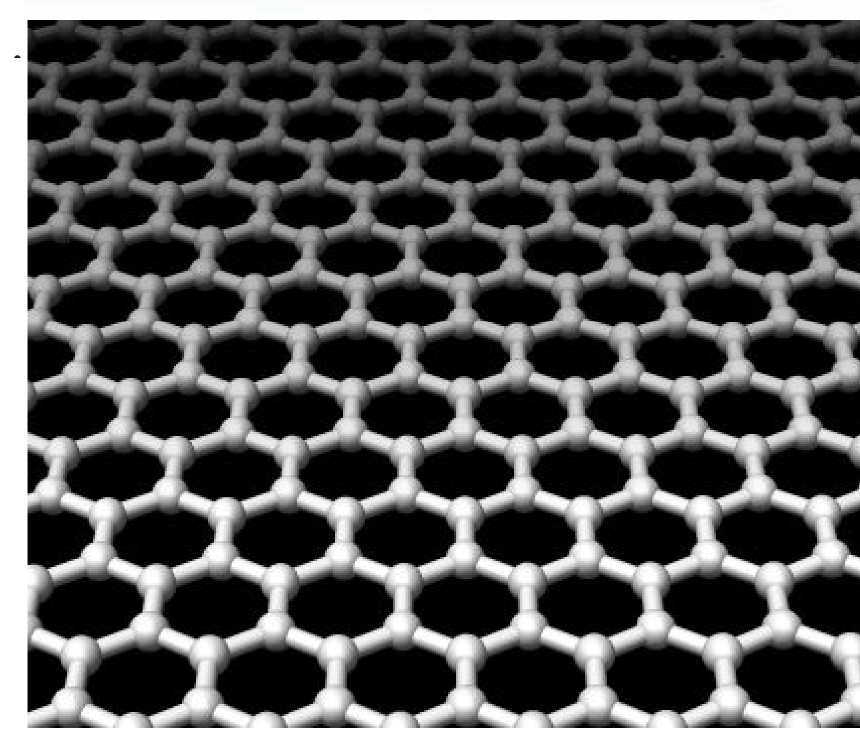




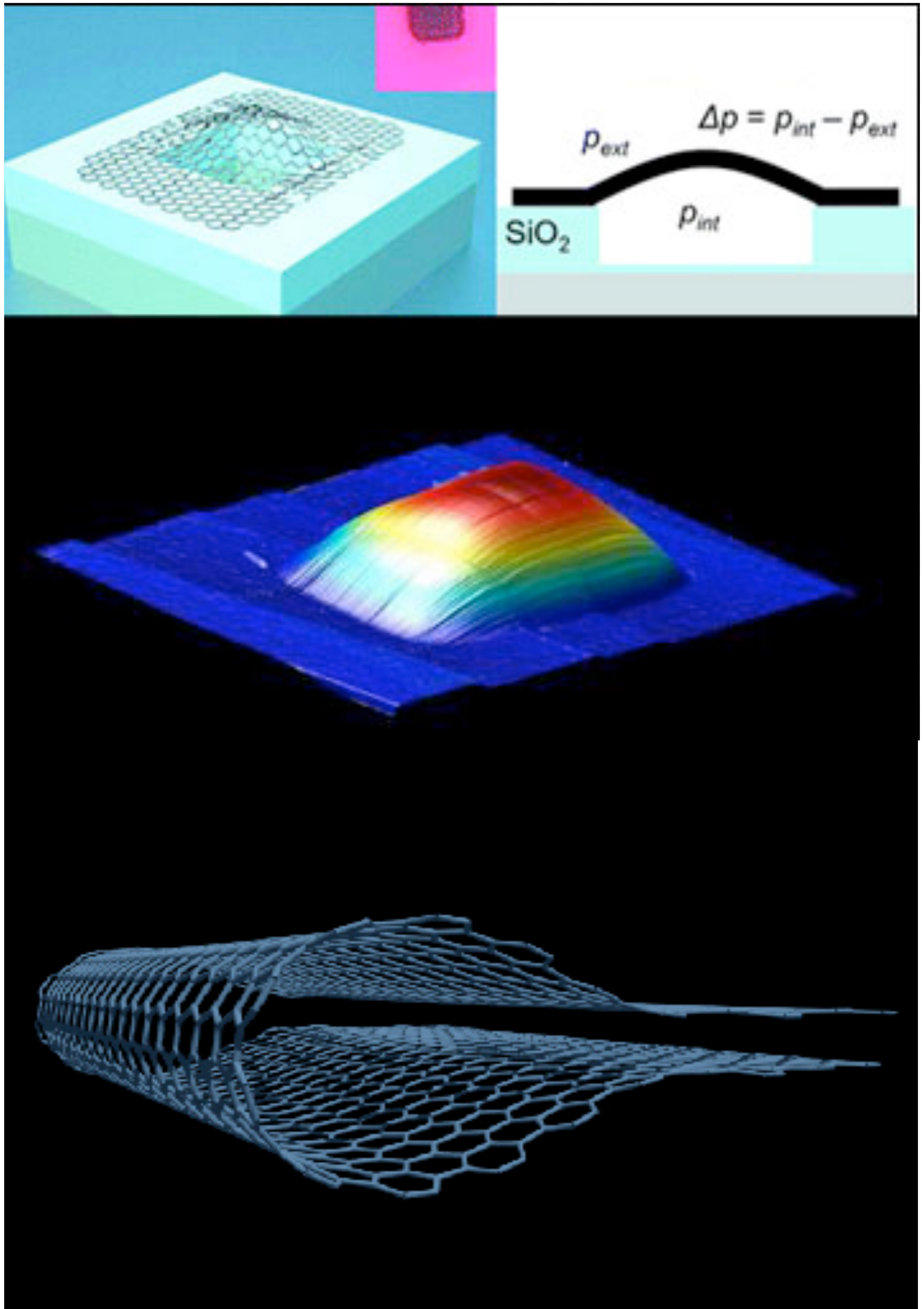

C. Lee et al., Science 321, 325 (2008)

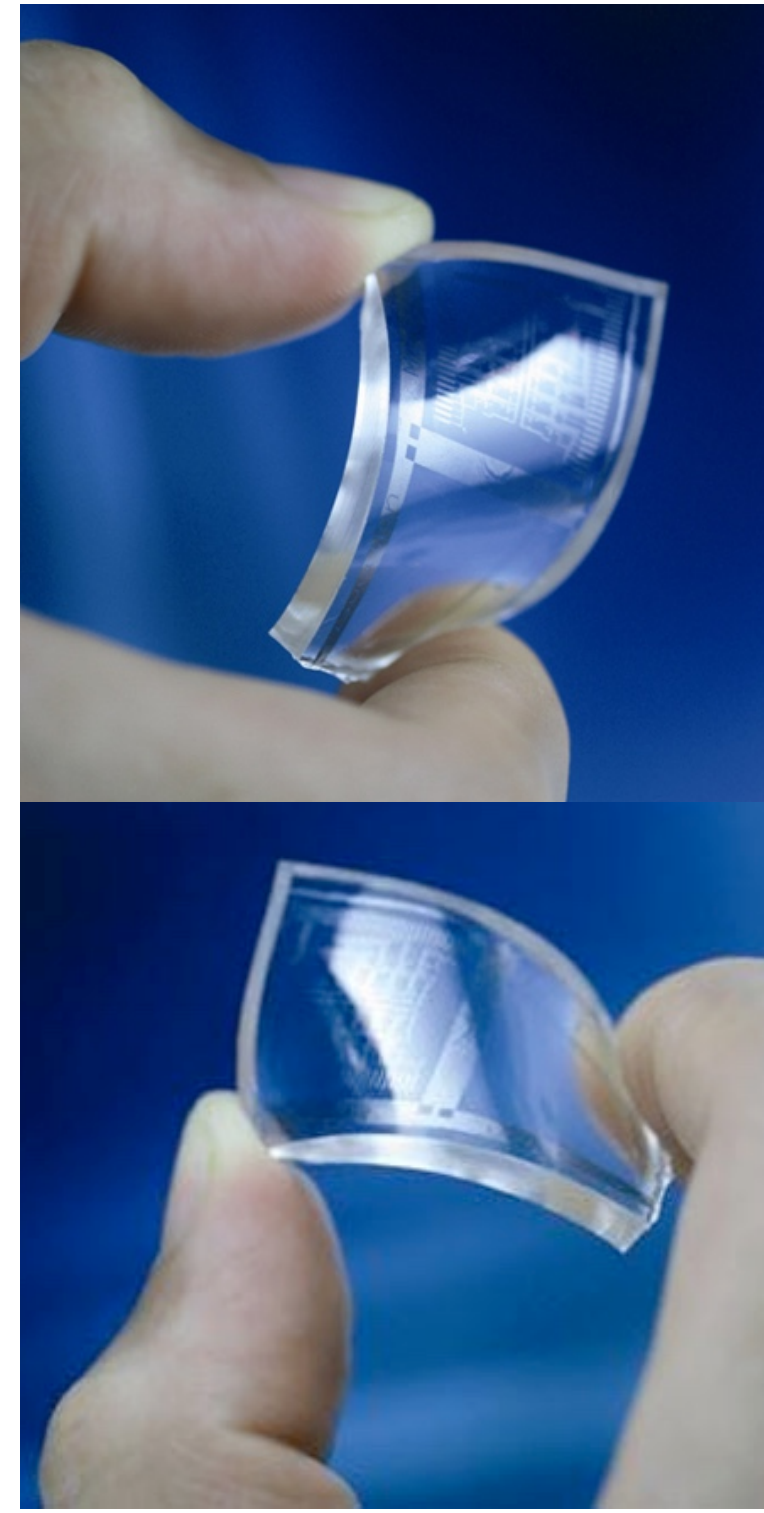


100 times stronger than the strongest steel!

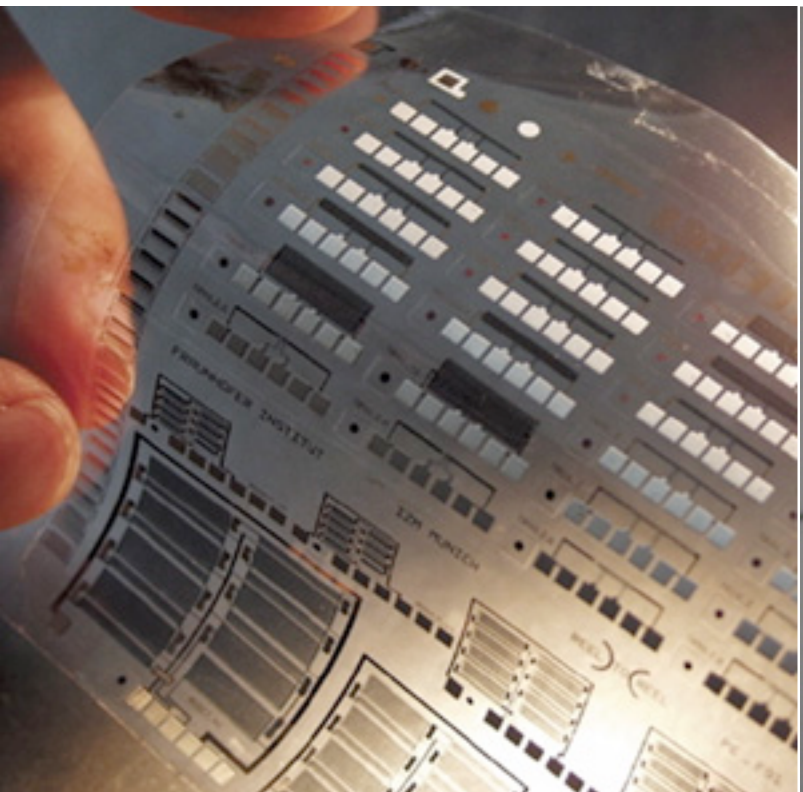
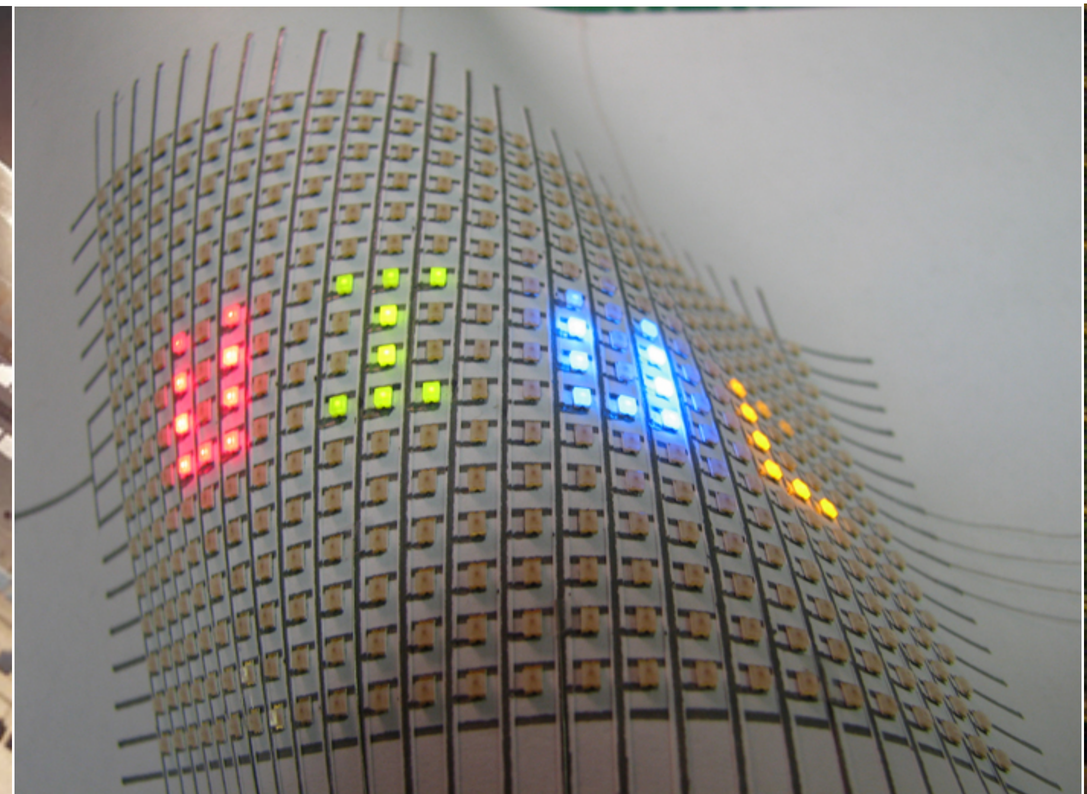
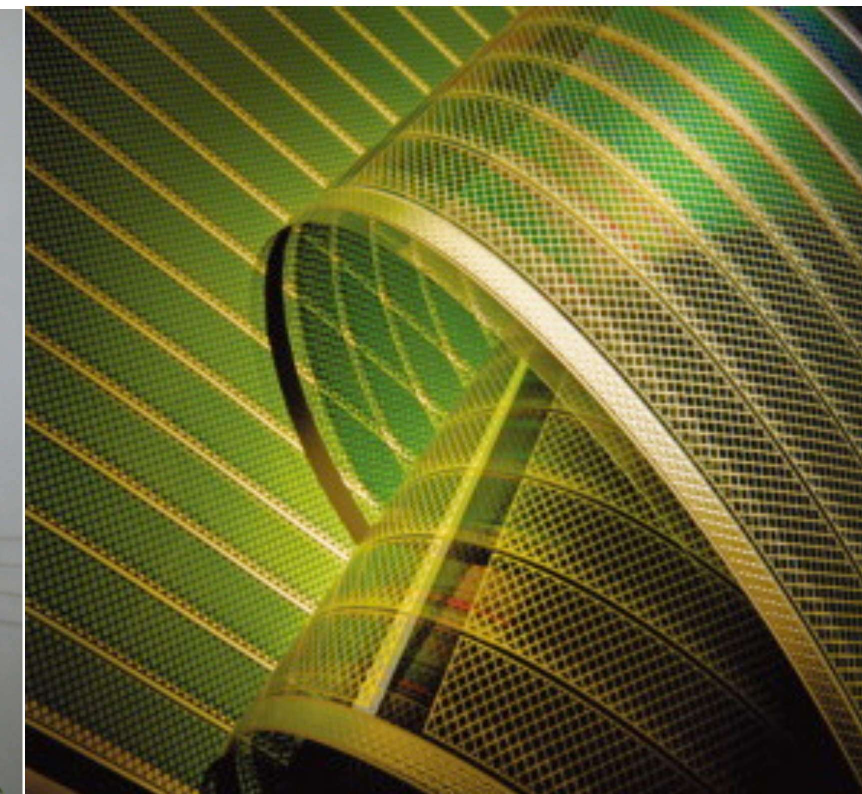
# Highly flexible

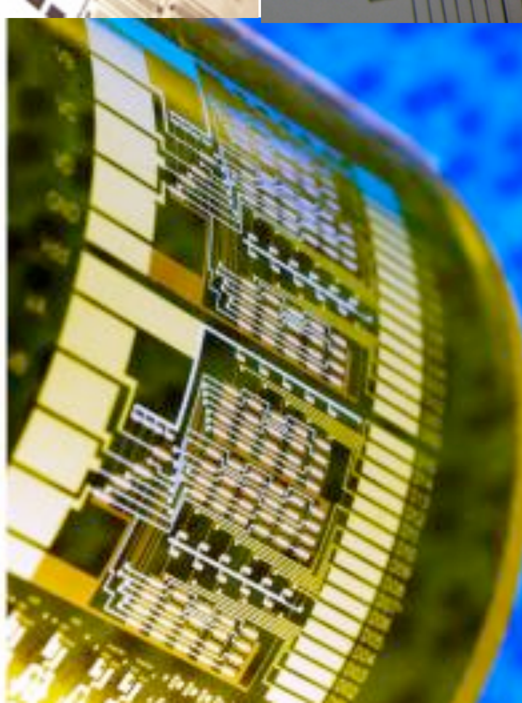
J. S. Bunch et al., Nano Lett. 8, 2458 (2008)

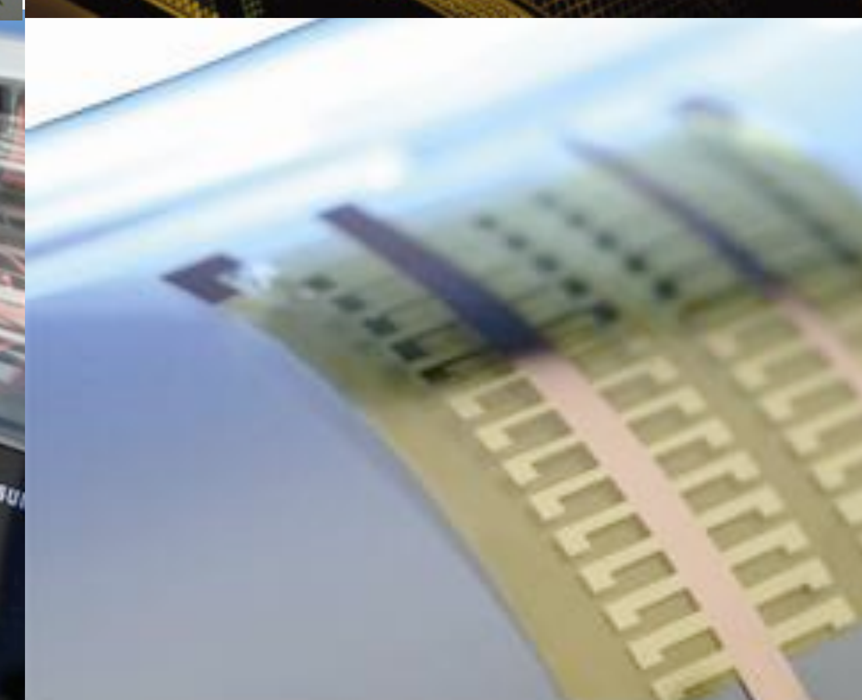


# Flexible electronics





# And much more...