Chair of Experimental Solid State Physics, LMU Munich

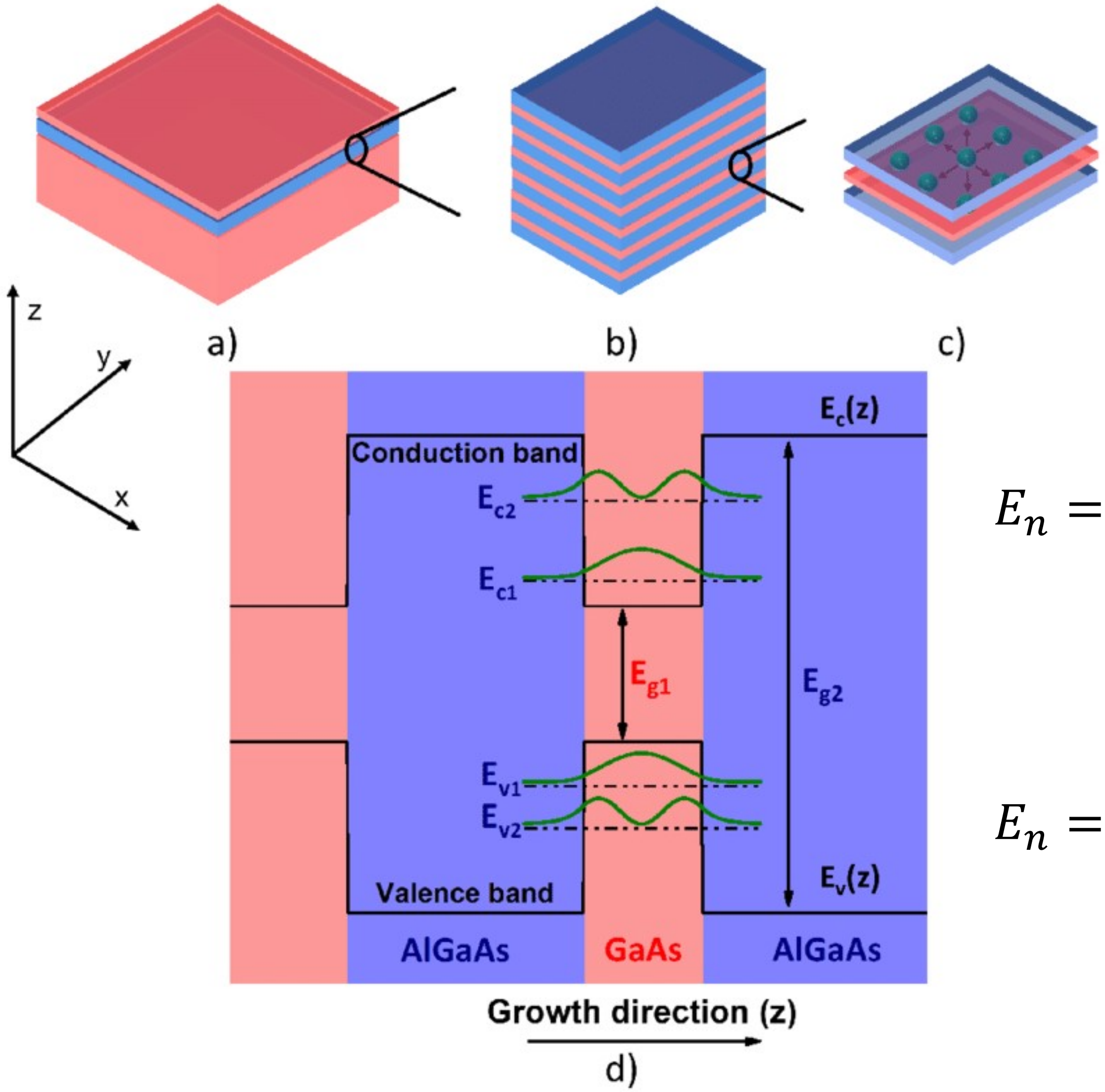
# “Introduction to Graphene and 2D Materials”

SS24 Lecture 9, 17/06/2024

# Outline - Lecture 9

- Band engineering with 1D and 2D super lattices and super potentials.
- Moiré patterns in graphene on hBN.
- Hofstadter butterfly in graphene on hBN.

# Quantum Wells




$$E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}$$

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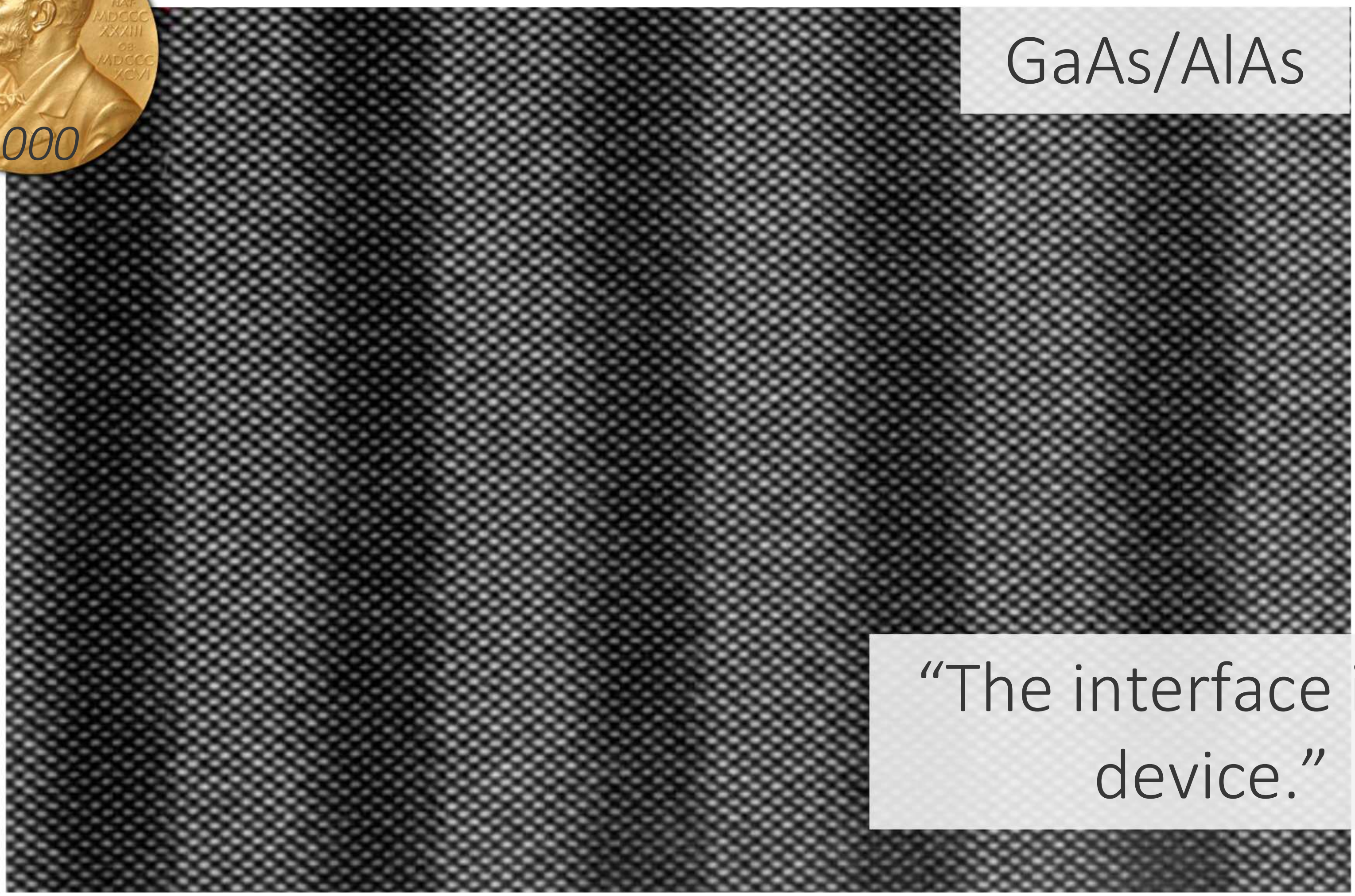
- By sandwiching a thin layer of semiconductor with another semiconductor with a straddling gap, one can create quantum wells, in which electrons are confined just like a particle in a box, and form bound states.

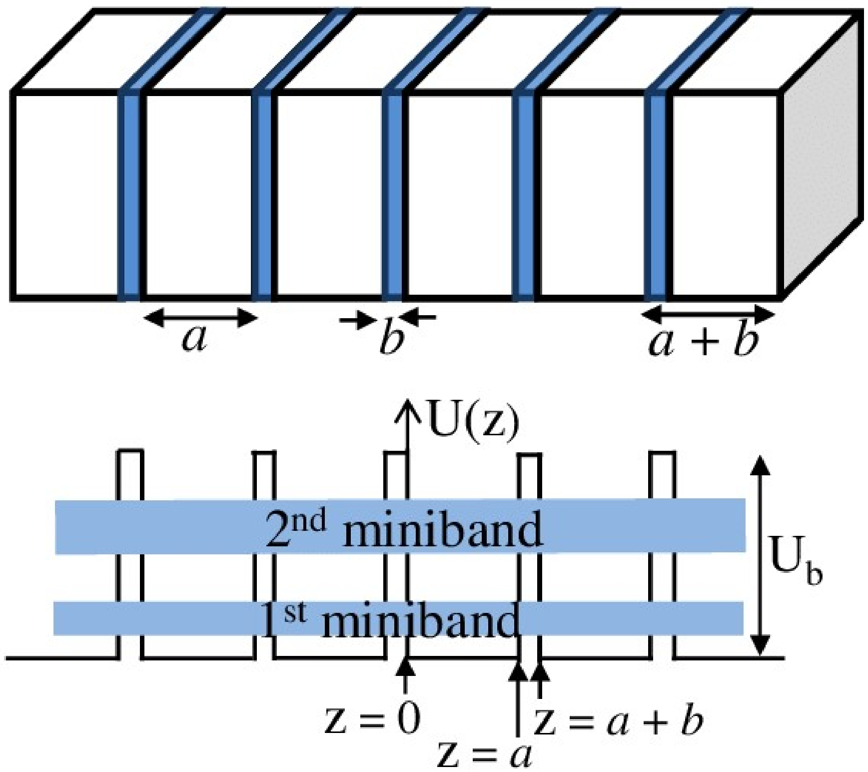
# Grown heterostructures – combining materials ’80

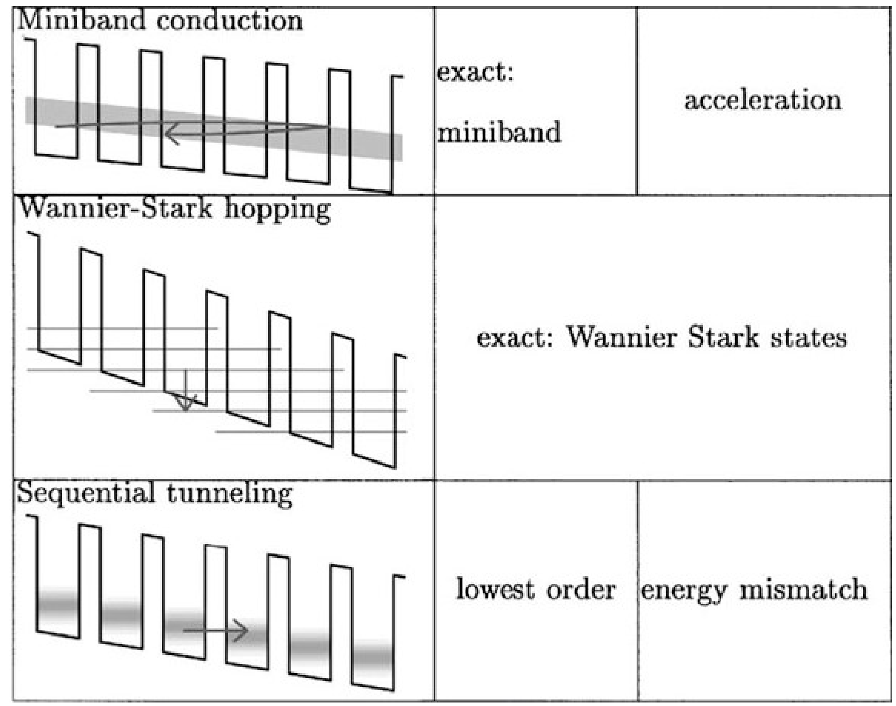

Semiconductor Heterostructure:




→ Combining materials with different properties
→ Interfaces rule

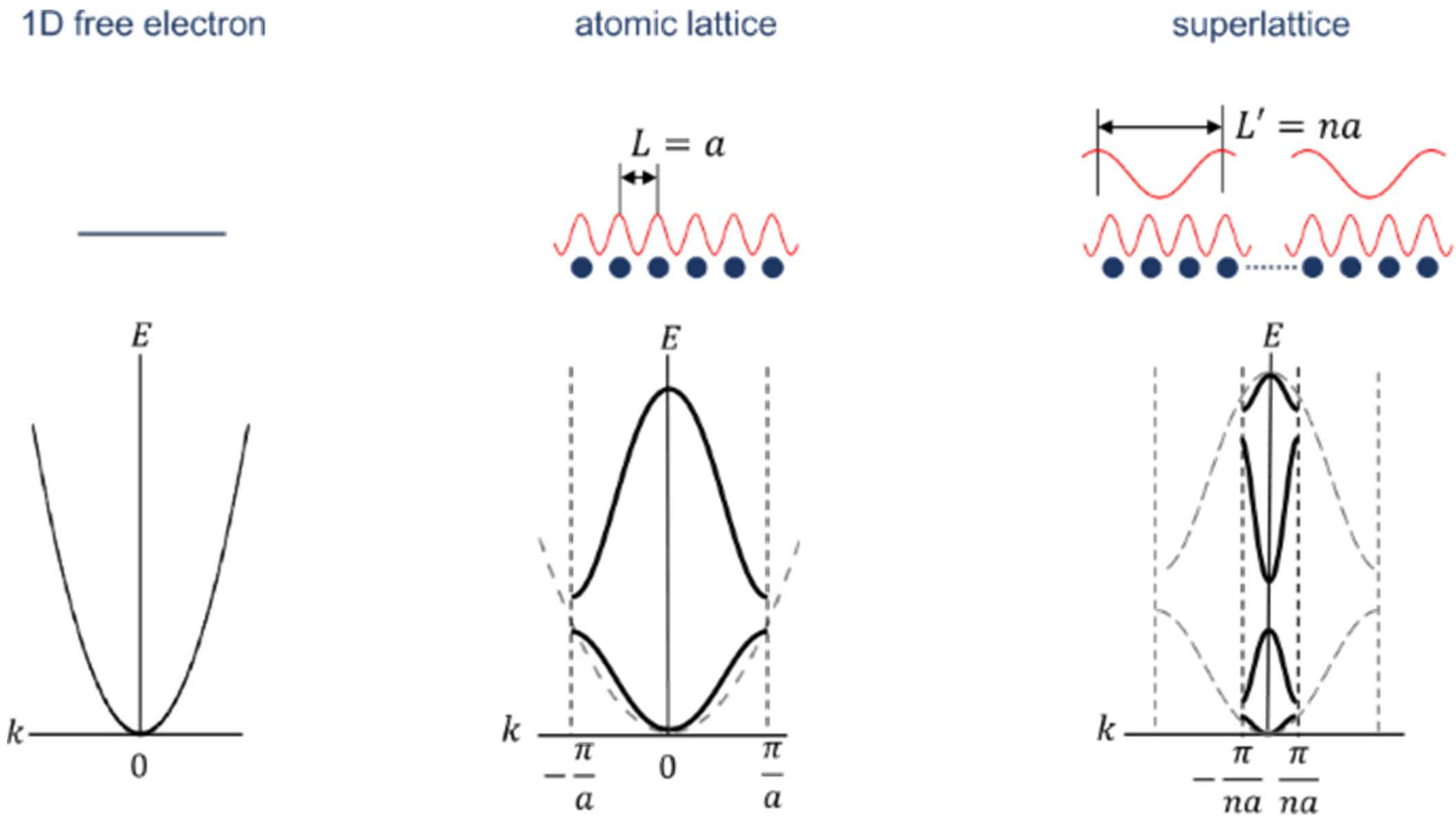
# 1D Superlattices




- A superlattice is a periodic structure of layers of two (or more) materials. Typically, the thickness of one layer is several nanometers. It can also refer to a lower-dimensional structure such as an array of quantum dots or quantum wells.
- For a high-mobility superlattice (mean free path >> superlattice constant) new Bloch states with a periodicity of the superlattice constant Z=a+b can be constructed.
- The superlattice gives rise to an enlarged unit cell and forms a new reduced mini-BZ with new mini-gaps arising at its boundaries.

# 1D Superlattice band-structure and mini-BZ

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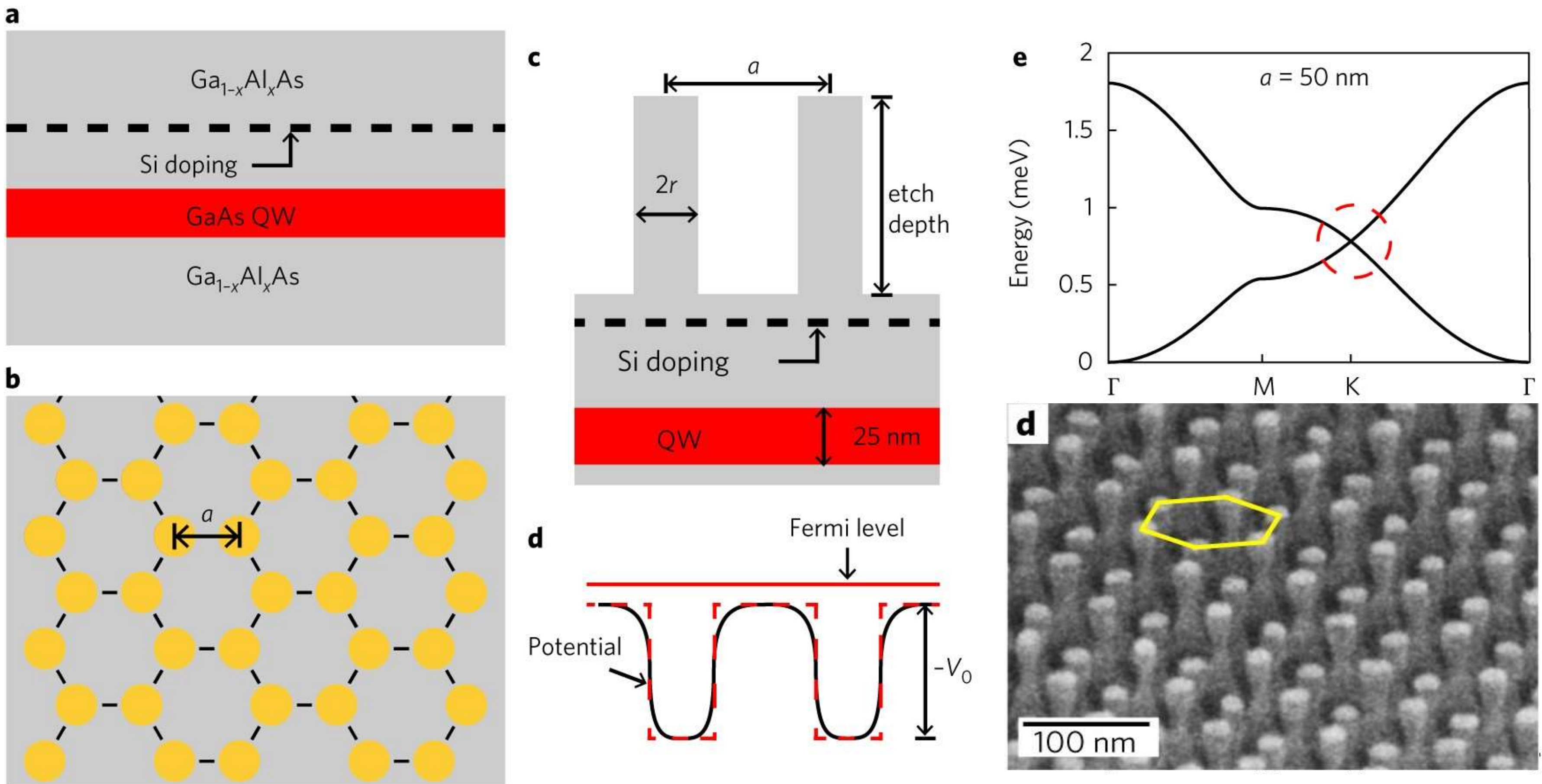
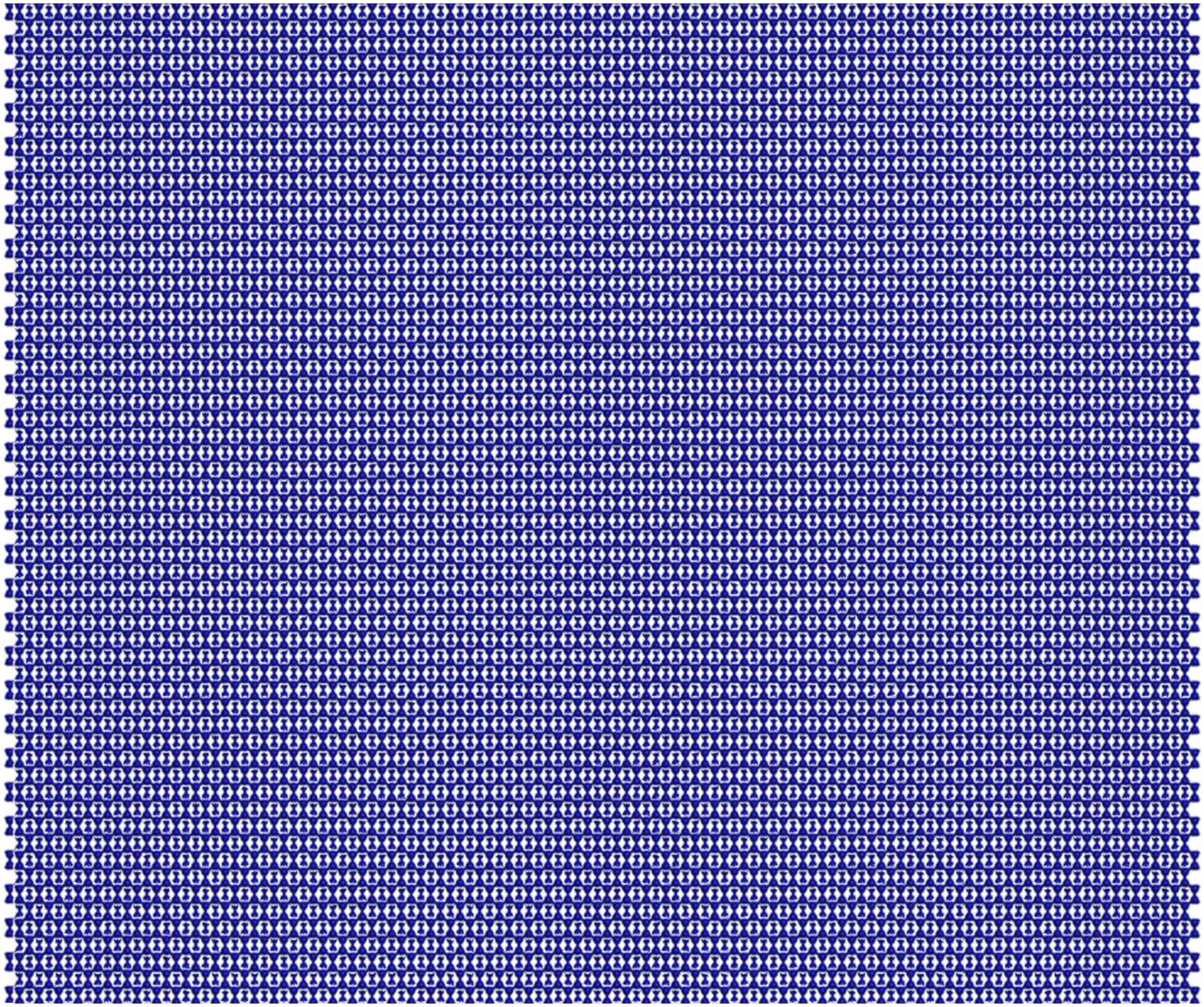
# Band structure engineering with superlattices



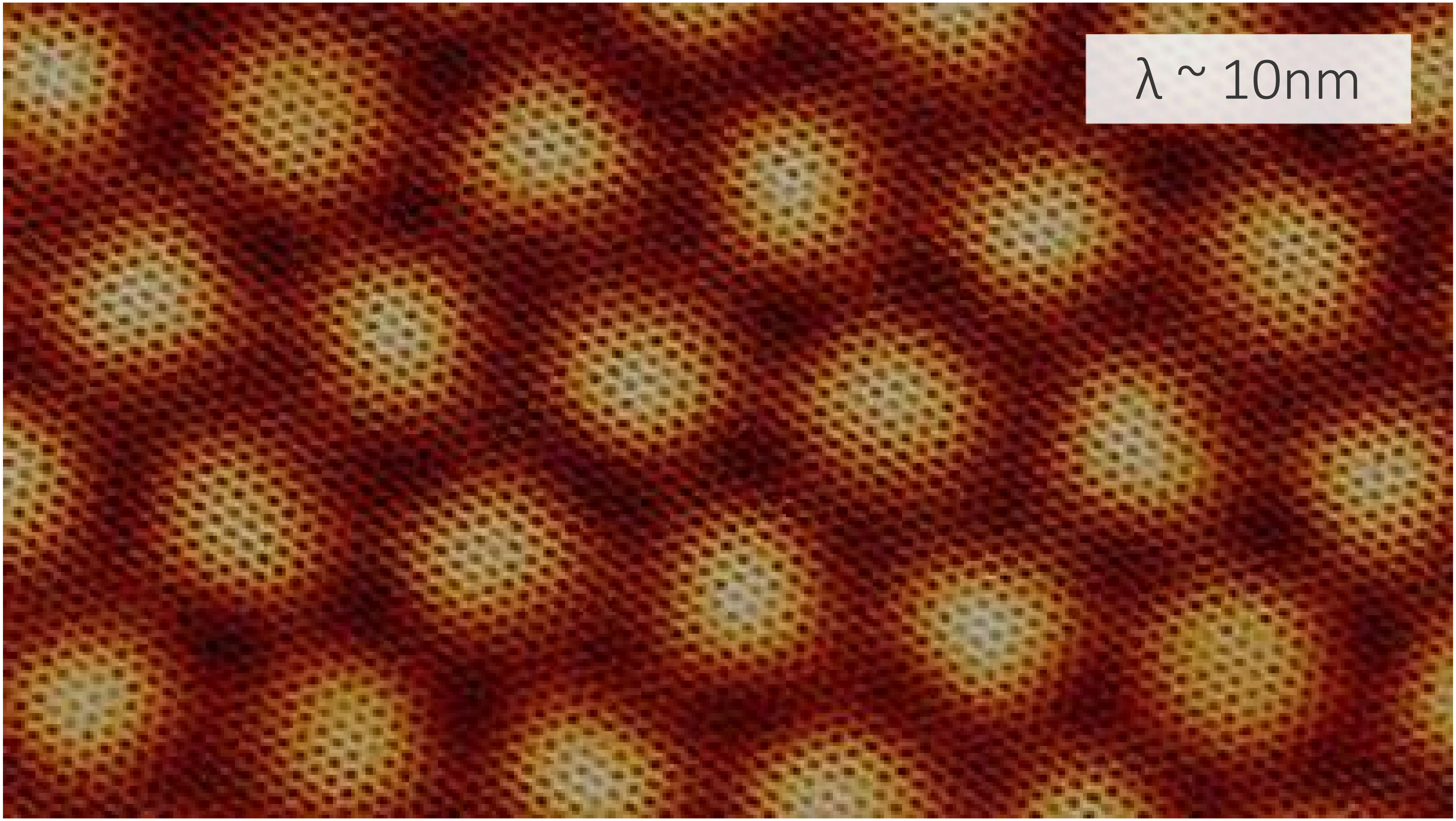

- Superlattice engineering offers a highly versatile platform to artificially engineer different band-structures with desired properties (topology, magnetism, superconductivity).
- F.e. one can construct a graphene band-structure in a semiconducting GaAs quantum well, by imposing a hexagonal superlattice on top of it.
- Problem → lithographically defined superlattices are disordered and it is hard to make small (<50nm) patterns.

# Twisting 2D materials – moiré superlattice



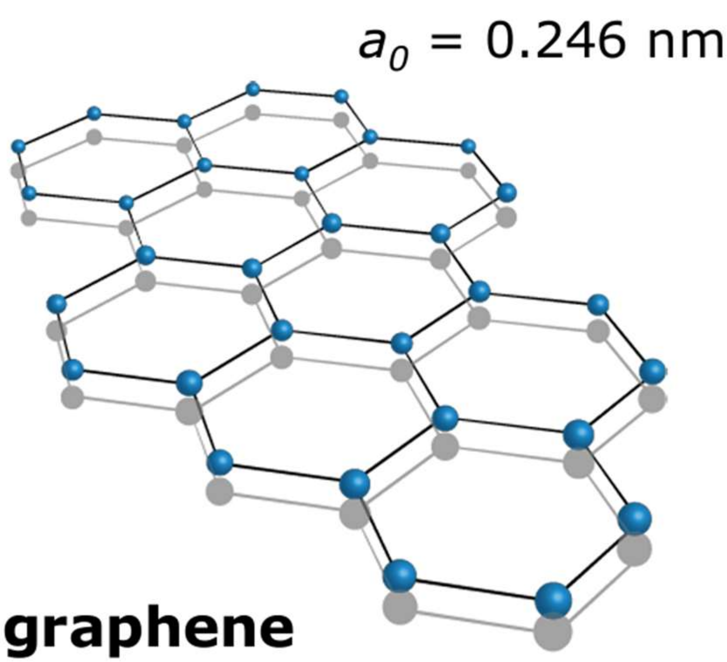
# Moire interference pattern – large scale superpotential

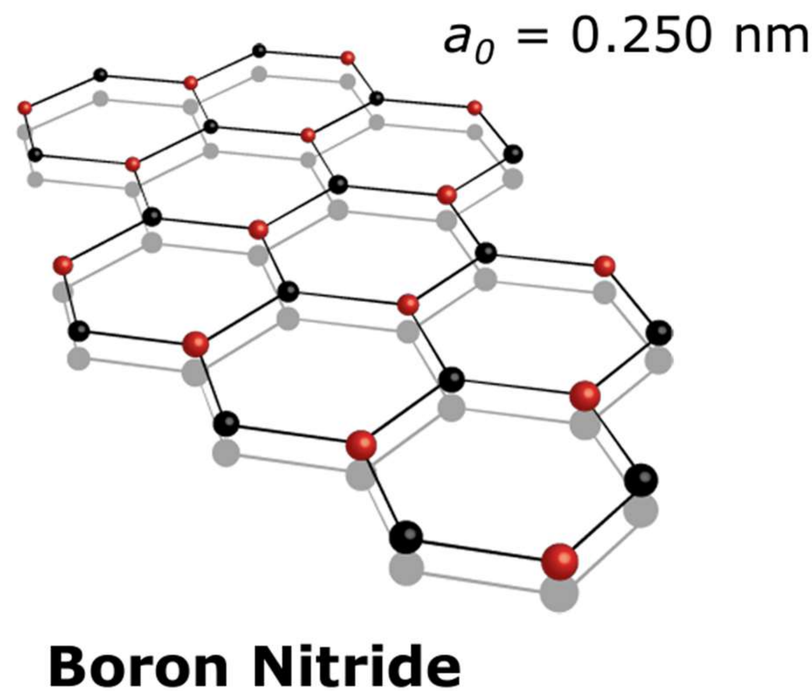
Scanning tunneling microscopy image of twisted bilayer graphene:




Yazdany group (2023).

# Graphene on hBN

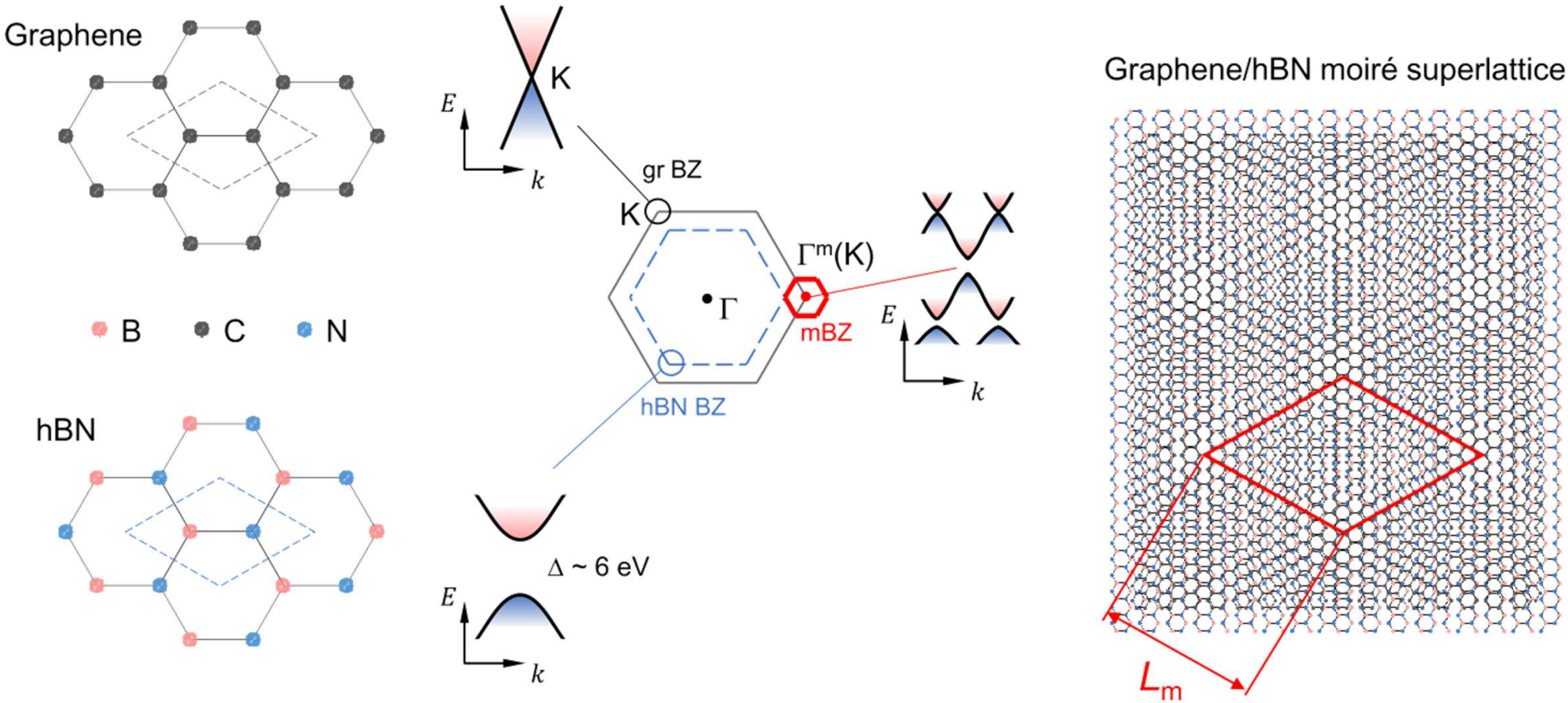



## Comparison of h-BN and $SiO_2$

| | Band Gap | Dielectric Constant | Optical Phonon Energy | Structure |
|---|---|---|---|---|
| BN | 5.5 eV | ~4 | >150 meV | Layered crystal |
| SiO2 | 8.9 eV | 3.9 | 59 meV | Amorphous |

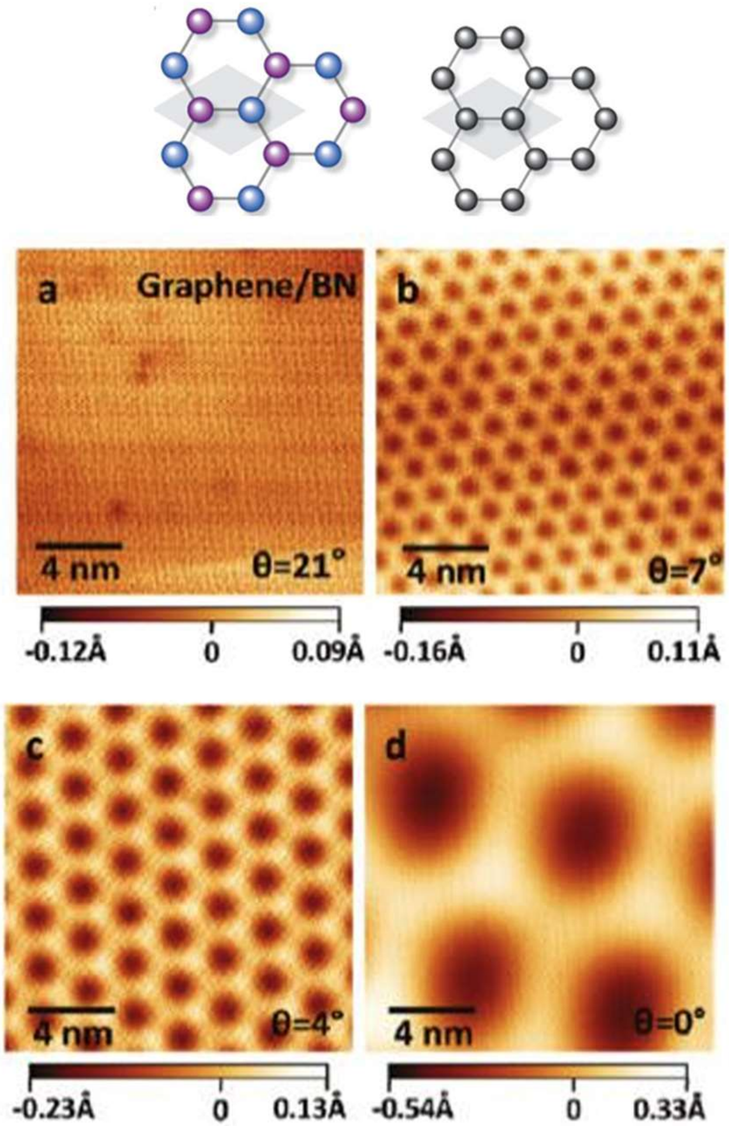
# Graphene on hBN - 2D Superlattice




- Graphene is a Dirac semi-metal with a lattice constant of 0.246nm.
- hBN is in insulator with a 6eV band-gap and a lattice constant of 0.250nm.
- Overlaying graphene with the hBN produces a moiré superlattice even at 0 degree twist angle and induces a new mini-BZ.
- The moiré super potential breaks the C2 symmetry of the graphene and induces a multitude of band-gaps.

# Moire patterns

Graphene on BN exhibits clear Moiré pattern

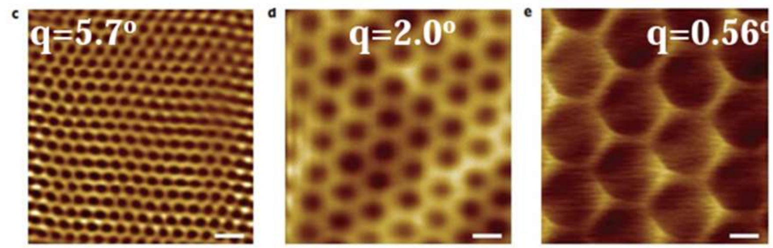


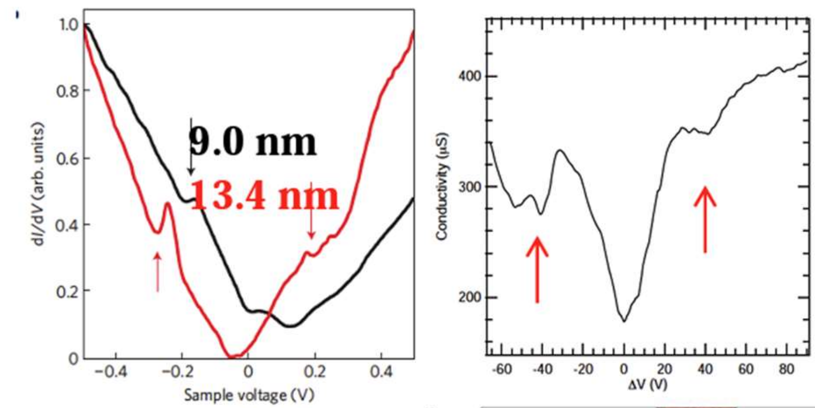

Xue et al, Nature Mater (2011);
Decker et al Nano Lett (2011)


LETTERS
PUBLISHED ONLINE: 25 MARCH 2012 | DOI: 10.1038/NPHYS2272
nature physics

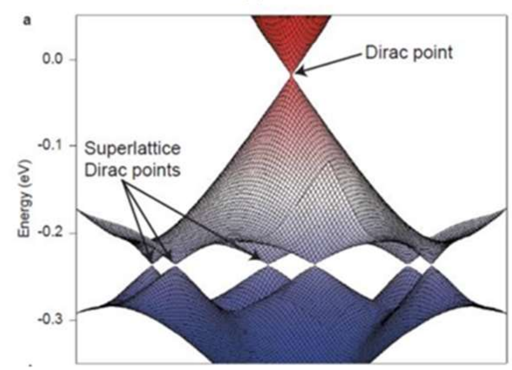

**Emergence of superlattice Dirac points in graphene on hexagonal boron nitride**


Matthew Yankowitz[1], Jiamin Xue[1], Daniel Cormode[1], Javier D. Sanchez-Yamagishi[2], K. Watanabe[3], T. Taniguchi[3], Pablo Jarillo-Herrero[2], Philippe Jacquod[1,4] and Brian J. LeRoy[1]*

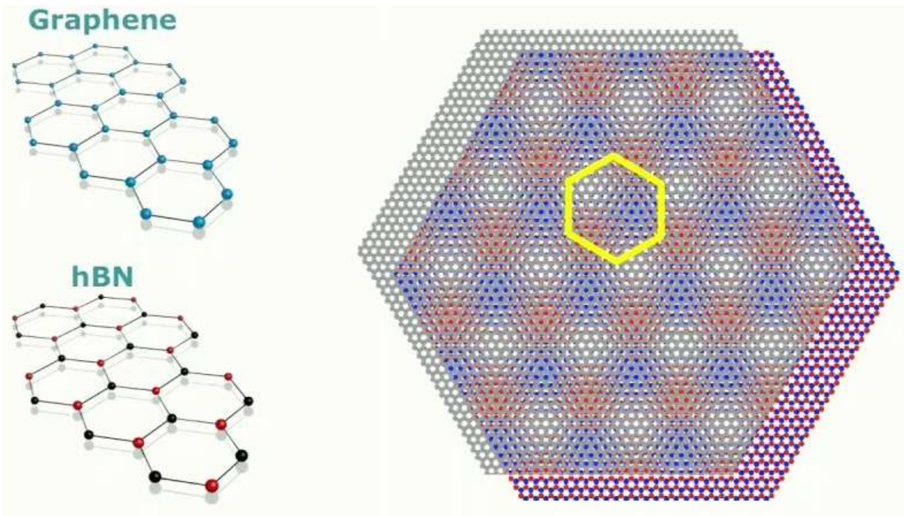




Minigap formation
near the Dirac point
due to Moire superlattice

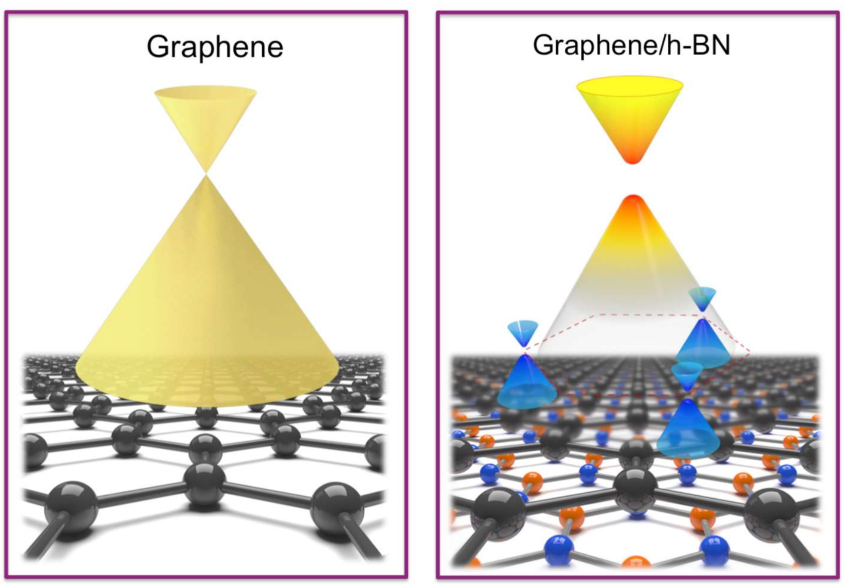


# Gaps through $C_2$ symmetry breaking with hBN

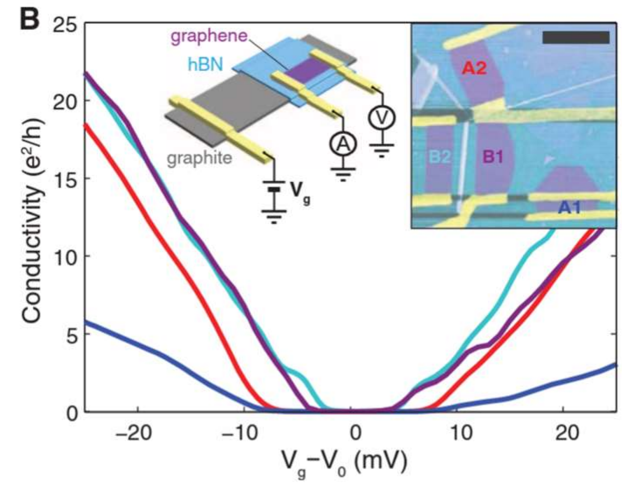
## Graphene on hBN – lattice mismatch:

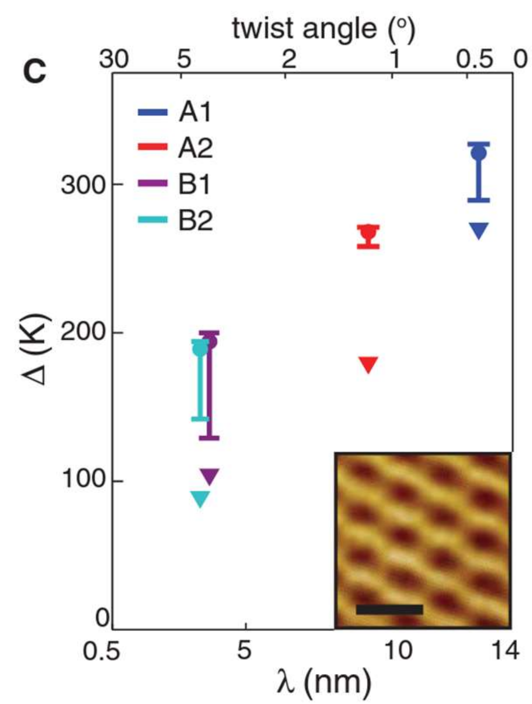



## Renormalized band-structure of Graphene on hBN:

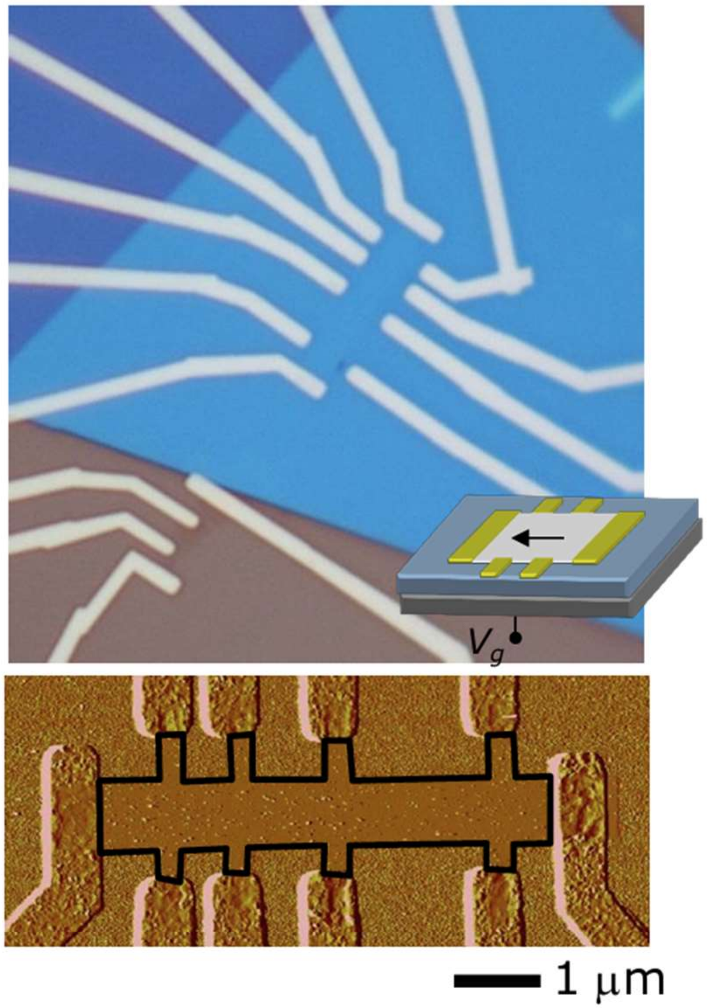


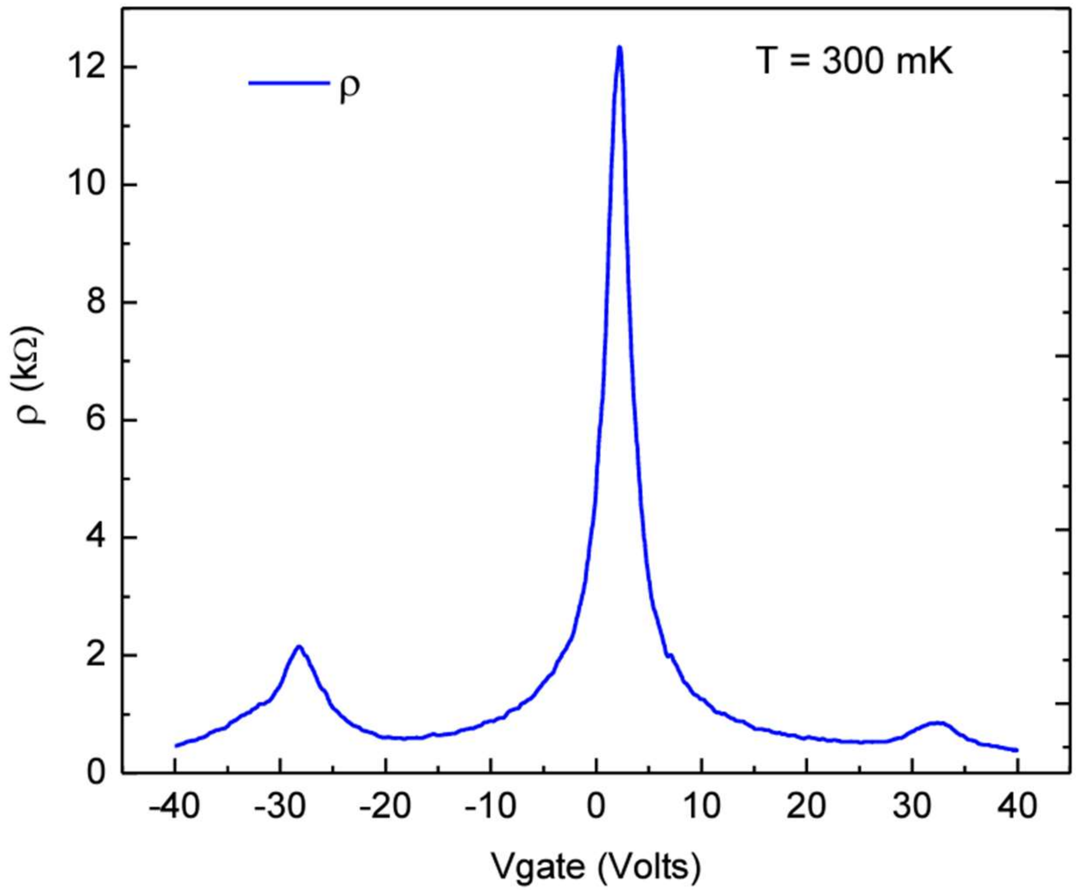

## Gapped Dirac cones on graphene/hBN:



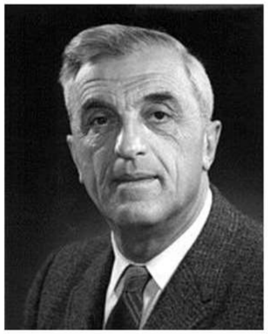
# Graphene/hBN transport properties




Bilayer graphene on BN substrates shows strong signature of satellite peaks…**some times… (~ 30%)**

# Bloch waves – Periodic waves



Felix Bloch

Zeitschrift für Physik, 52, 555 (1929)

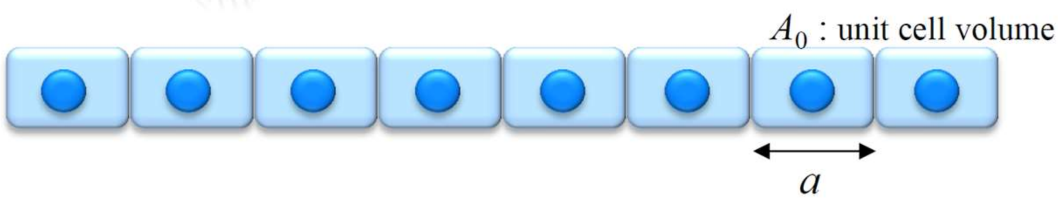
**Über die Quantenmechanik der Elektronen in Kristallgittern.**

Von **Felix Bloch** in Leipzig.

Mit 2 Abbildungen. (Eingegangen am 10. August 1928.)

## Periodic Lattice

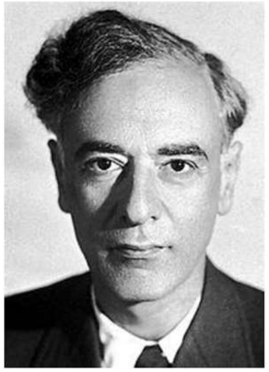
$$\tilde{H} = \frac{\tilde{p}^2}{2m} + U(x), \qquad U(x) = U(x+a)$$




## Block Waves:

$$\psi_{n,k}(x) = e^{ikx} u_{n,k}(x), \qquad u_{n,k}(x+a) = u_{n,k}(x)$$

# Landau Levels – Cyclotron Orbits



Lev Landau

Zeitschrift für Physik, 64, 629 (1930)

**Diamagnetismus der Metalle.**

Von **L. Landau**, zurzeit in Cambridge (England).

(Eingegangen am 25. Juli 1930.)

Free electron under magnetic field

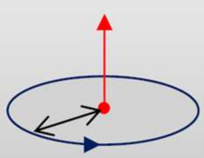
$$\tilde{H} = \frac{(\tilde{\mathrm{p}} - e\mathbf{A}/c)^2}{2m}$$

Energy and orbit are quantized:

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

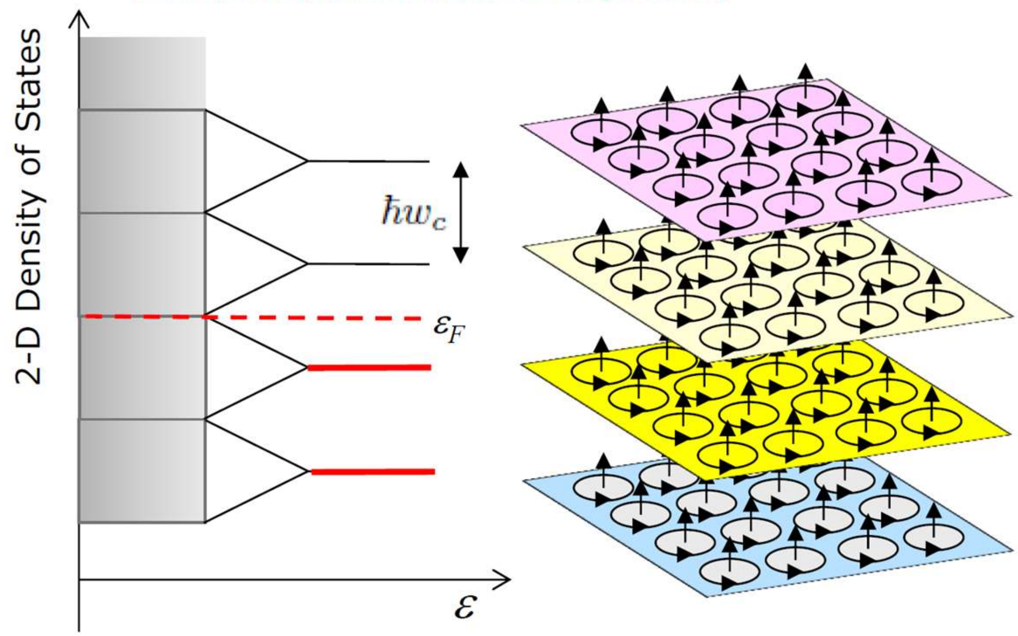
Each Landau orbit contains magnetic flux quanta

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



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

**2-dimensional electron systems**




Massively degenerated energy level

Landau level filling fraction:

$$\nu = 2\pi\ell_B^2 n(\varepsilon_F)$$

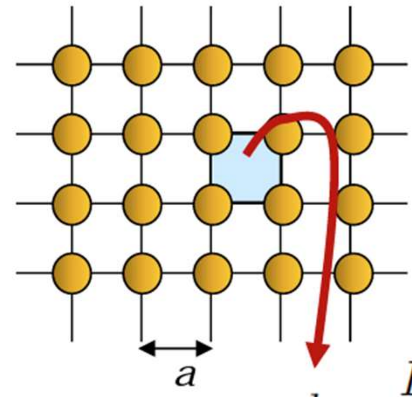
# Harpers equation – competition of two length scales

Proc. Phys. Soc. Lond. A 68 879 (1955) 879

**The General Motion of Conduction Electrons in a Uniform Magnetic Field, with Application to the Diamagnetism of Metals**

By P. G. HARPER†
Department of Mathematical Physics, University of Birmingham

*Communicated by R. E. Peierls; MS. received 19th January 1955 and in amended form 27th April 1955*




$$b = \frac{Ba^2}{\phi_0} = \frac{\phi}{\phi_0}$$

**Tight binding on 2D Square lattice with magnetic field**

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

Two competing length scales:

$a$ **: lattice periodicity**

$l_B$ **: magnetic periodicity**

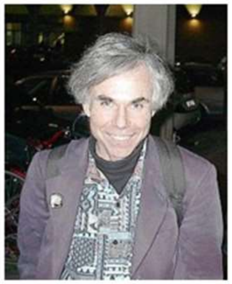
**Harper's Equation**

$$2\psi_l \cos(2\pi l b - \kappa) + \psi_{l+1} + \psi_{l-1} = E\psi_l$$

For $b \ll \mu^* H$, the broadening factor may be written approximately $\exp[-(bv\pi/\mu^* H)^2]$ and the broadening effect becomes additive to that due to collision as described by Dingle (1952 b).

The level structure in the vicinity of an energy gap near a zone boundary is all-important for the de Haas–van Alphen effect. Unfortunately, this seems very difficult to determine in detail, even for a sinusoidal potential. Apart from the regularity already mentioned there seems little one can say. It is likely, however, that if periodicity exists, the period will give rise to effective mass parameters much smaller than one would otherwise expect. This is because the level structure will consist of irregular groups, regularly repeated. Since the period is large, the oscillatory period will also be large and the effective mass correspondingly smaller.

# Hofstadters butterfly



PHYSICAL REVIEW B VOLUME 14, NUMBER 6 15 SEPTEMBER 1976

**Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields***

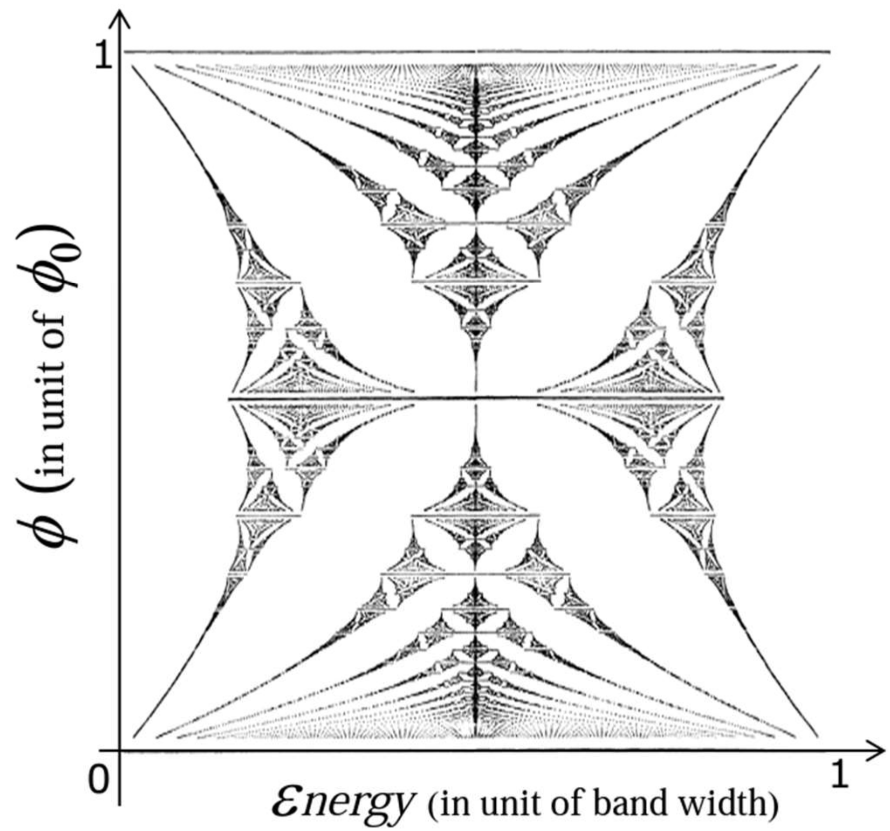
Douglas R. Hofstadter†
*Physics Department, University of Oregon, Eugene, Oregon 97403*
(Received 9 February 1976)

Harper's Equation

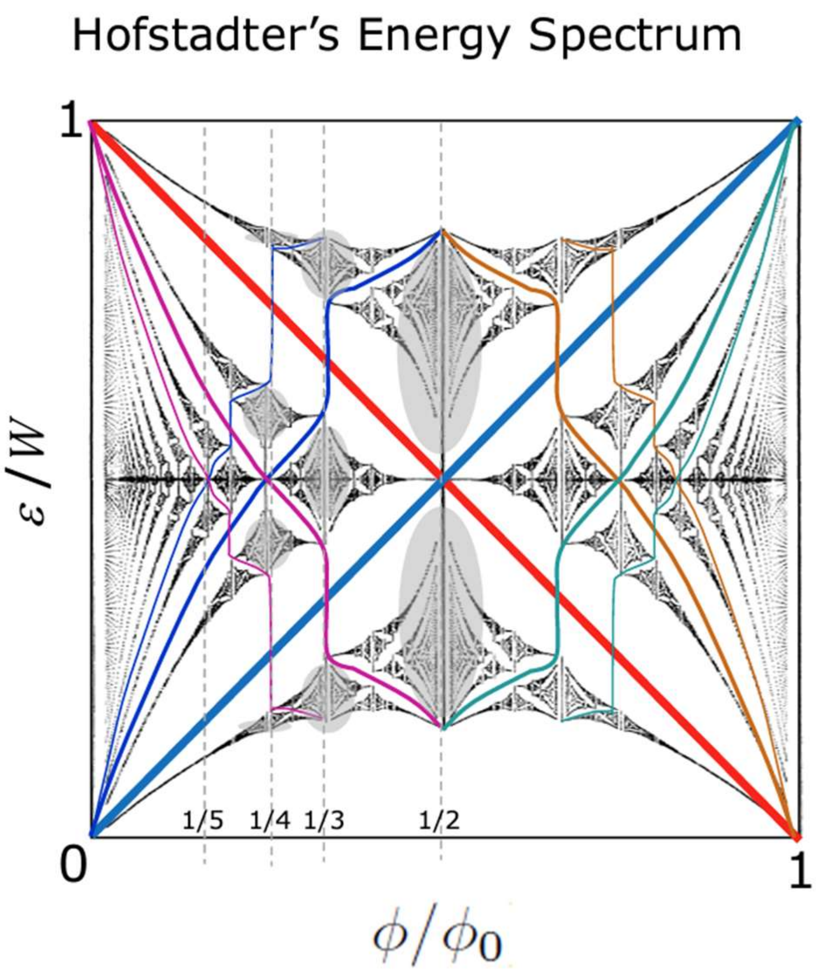
$$2\psi_l \cos\left(2\pi l b - \kappa\right) + \psi_{l+1} + \psi_{l-1} = E\psi_l$$

When $b=p/q$, where $p$, $q$ are coprimes, each LL splits into ***q sub-bands that are p-fold degenerate***

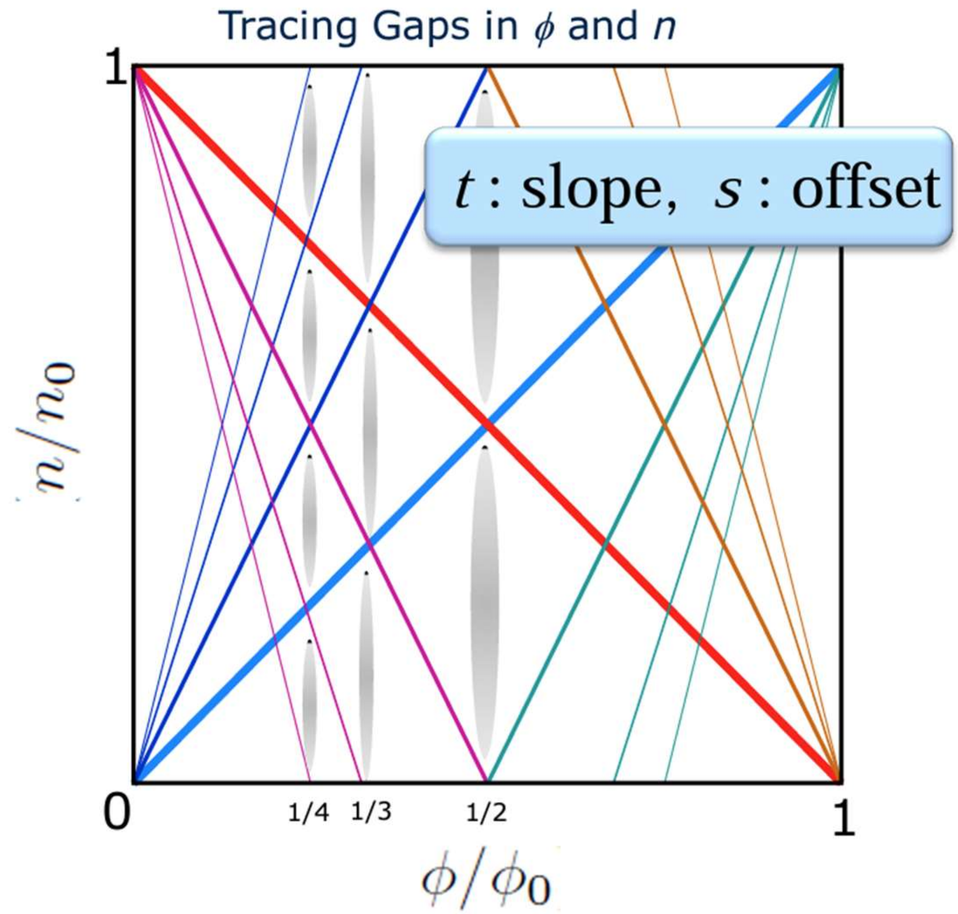
Energy bands develop ***fractal structure*** when magnetic length is of order the periodic unit cell



# Wannier diagram




Wannier, *Phys. Status Solidi.* **88**, 757 (1978)

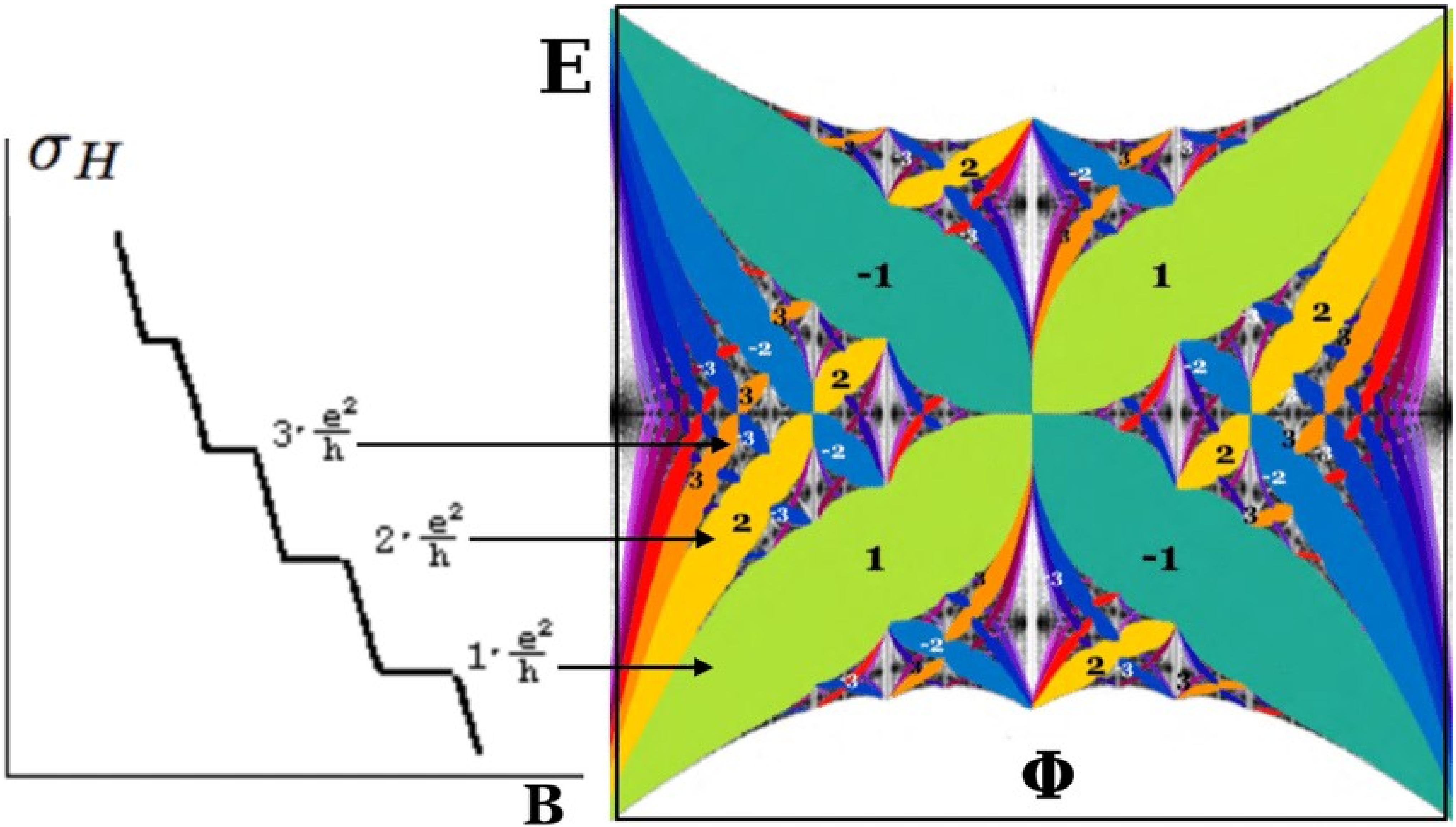



$n_0$: # of state per unit cell
$\phi$ : magnetic flux in unit cell
$n$ : electron density

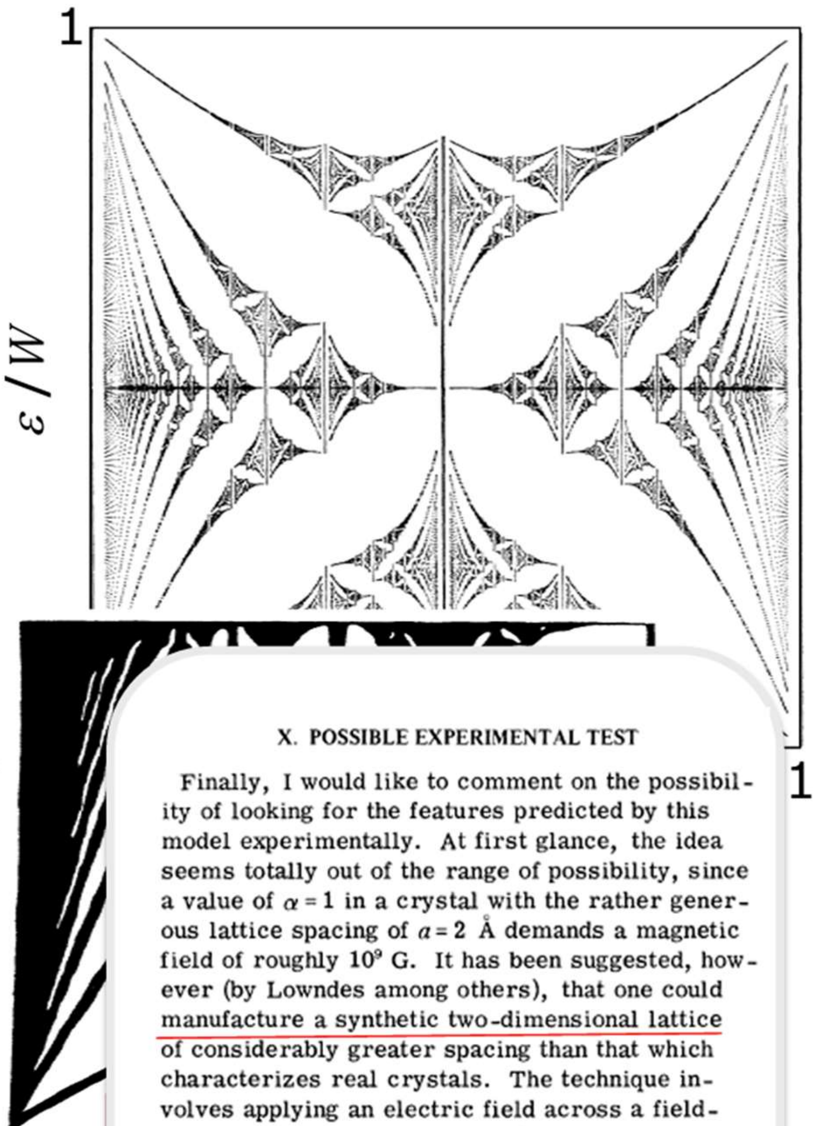
**Diophantine equation for gaps**

$$(n/n_0) = t(\phi/\phi_0) + s \qquad t, s \in \mathbb{Z}$$

# Hofstadters butterfly



# Experimental challenge



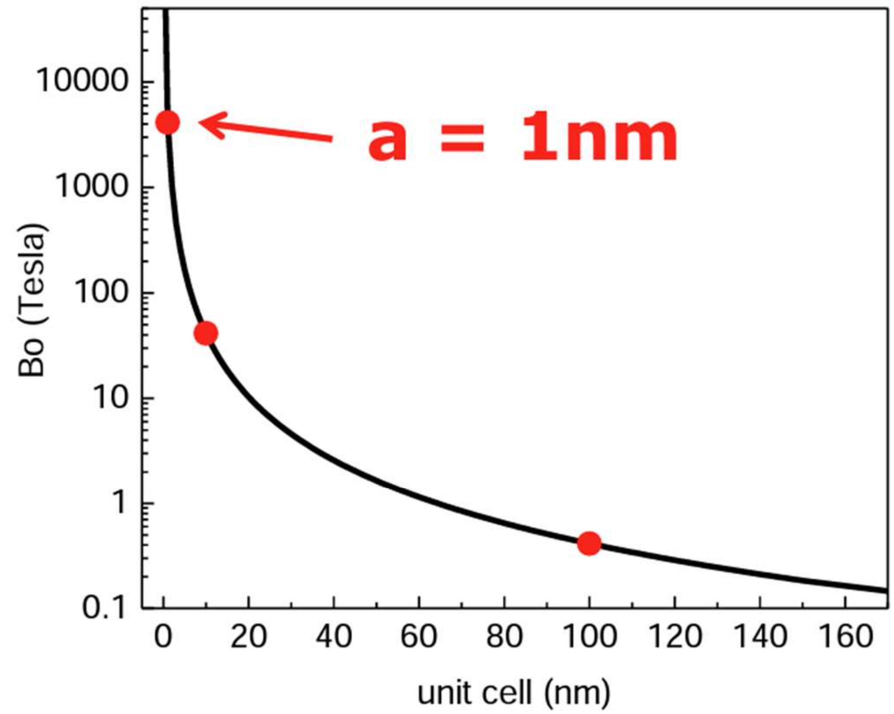

X. POSSIBLE EXPERIMENTAL TEST

Finally, I would like to comment on the possibility of looking for the features predicted by this model experimentally. At first glance, the idea seems totally out of the range of possibility, since a value of $\alpha = 1$ in a crystal with the rather generous lattice spacing of $a = 2$ Å demands a magnetic field of roughly $10^9$ G. It has been suggested, however (by Lowndes among others), that one could manufacture a synthetic two-dimensional lattice of considerably greater spacing than that which characterizes real crystals. The technique involves applying an electric field across a field-effect transistor (without leads). The effect of

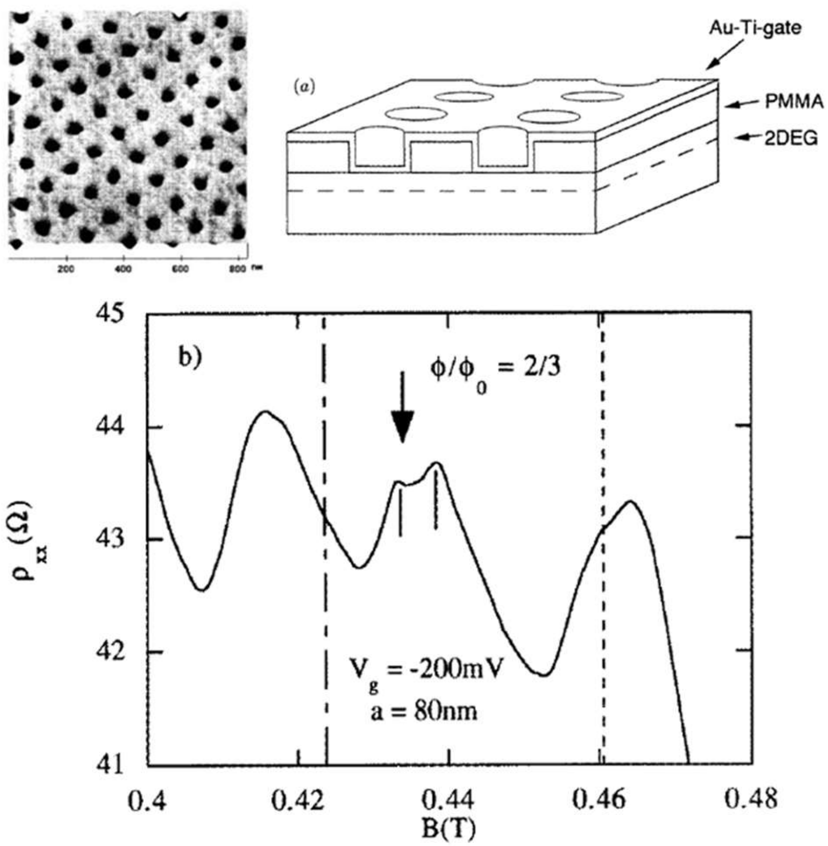
Hofstadter (1976)

**Obvious technical challenge:**

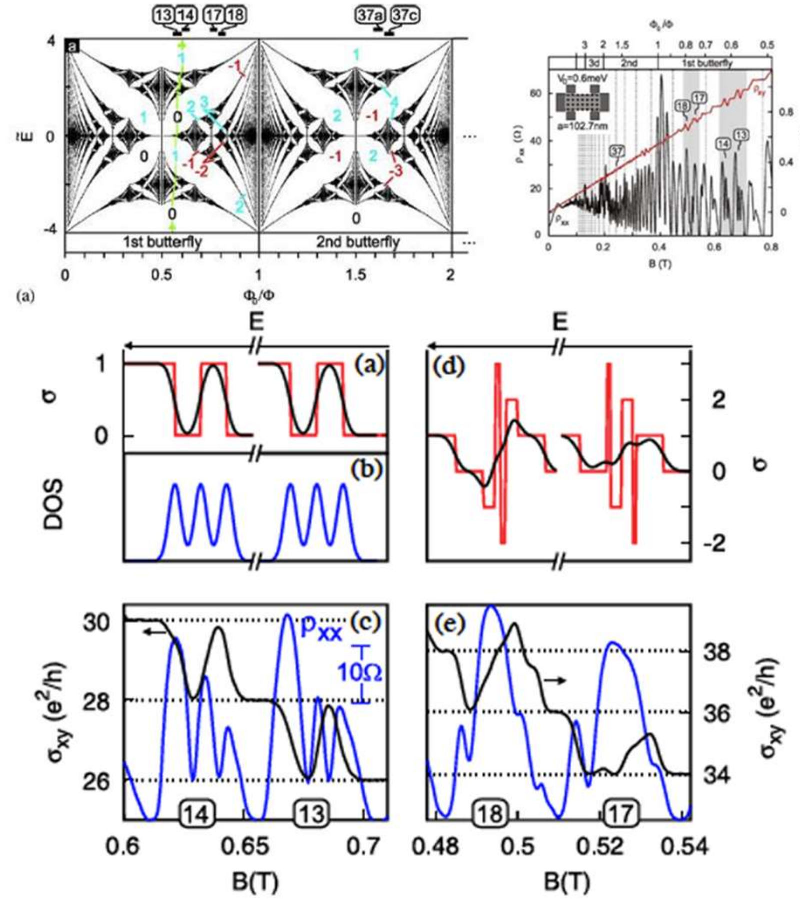
$$\frac{\phi}{\phi_o} = \frac{Ba^2}{h/e} \sim 1$$



# Search for Hofstadter butterfly




-Schlosser et al, Semicond. Sci. Technol. (1996)



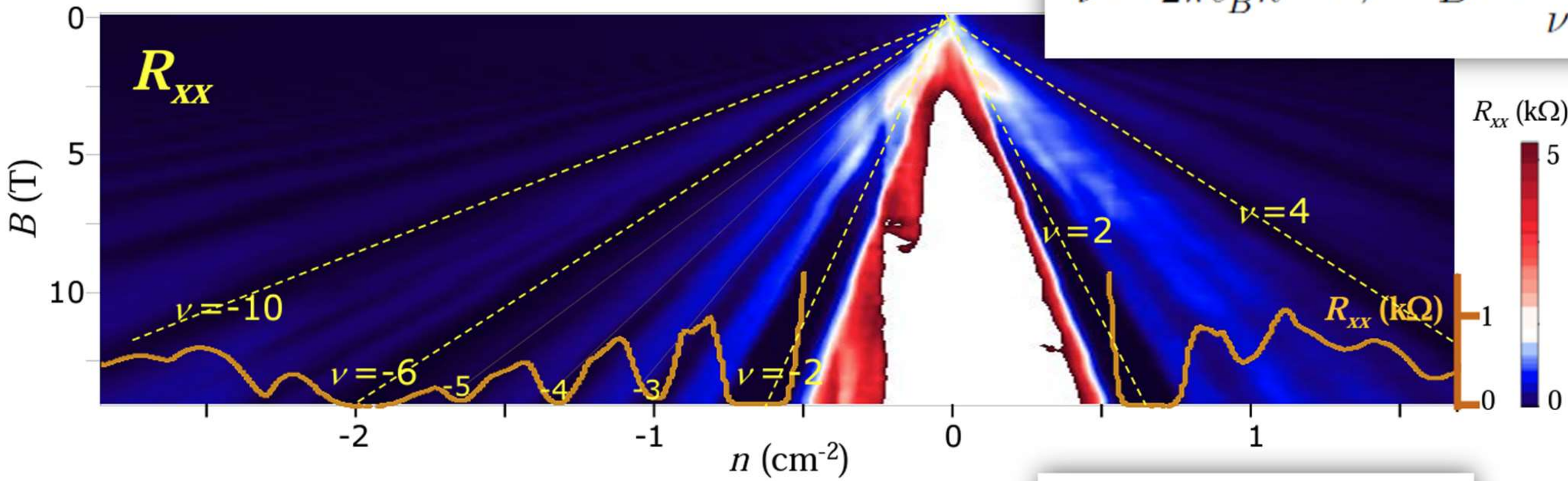

Albrecht et al, PRL. (2001);
Geisler et al, PRL (2004)

- Unit cell limited to ~100 nm
- limited field and density range accessible, weak perturbation
- Do not observe ‘fully quantized’ mingaps in fractal spectrum

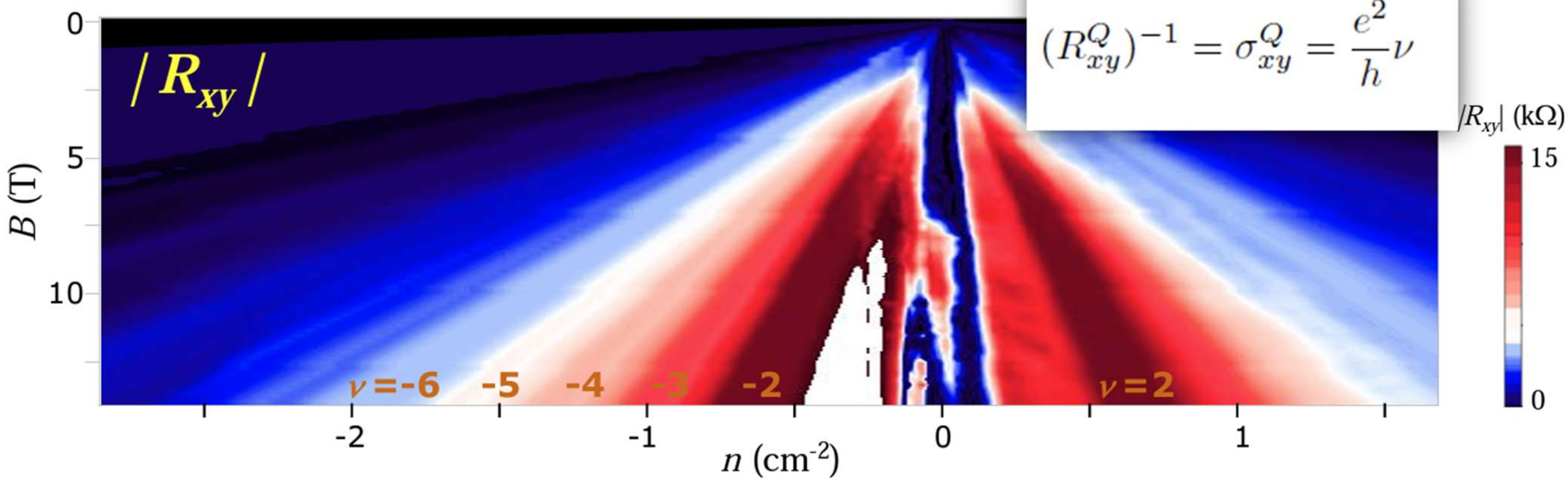
# Normal graphene QHE fan diagram

## Landau Fan Diagram for "typical" graphene

$$\nu = 2\pi \ell_B^2 n \quad \Rightarrow \quad B = \frac{\phi_0}{\nu} n$$



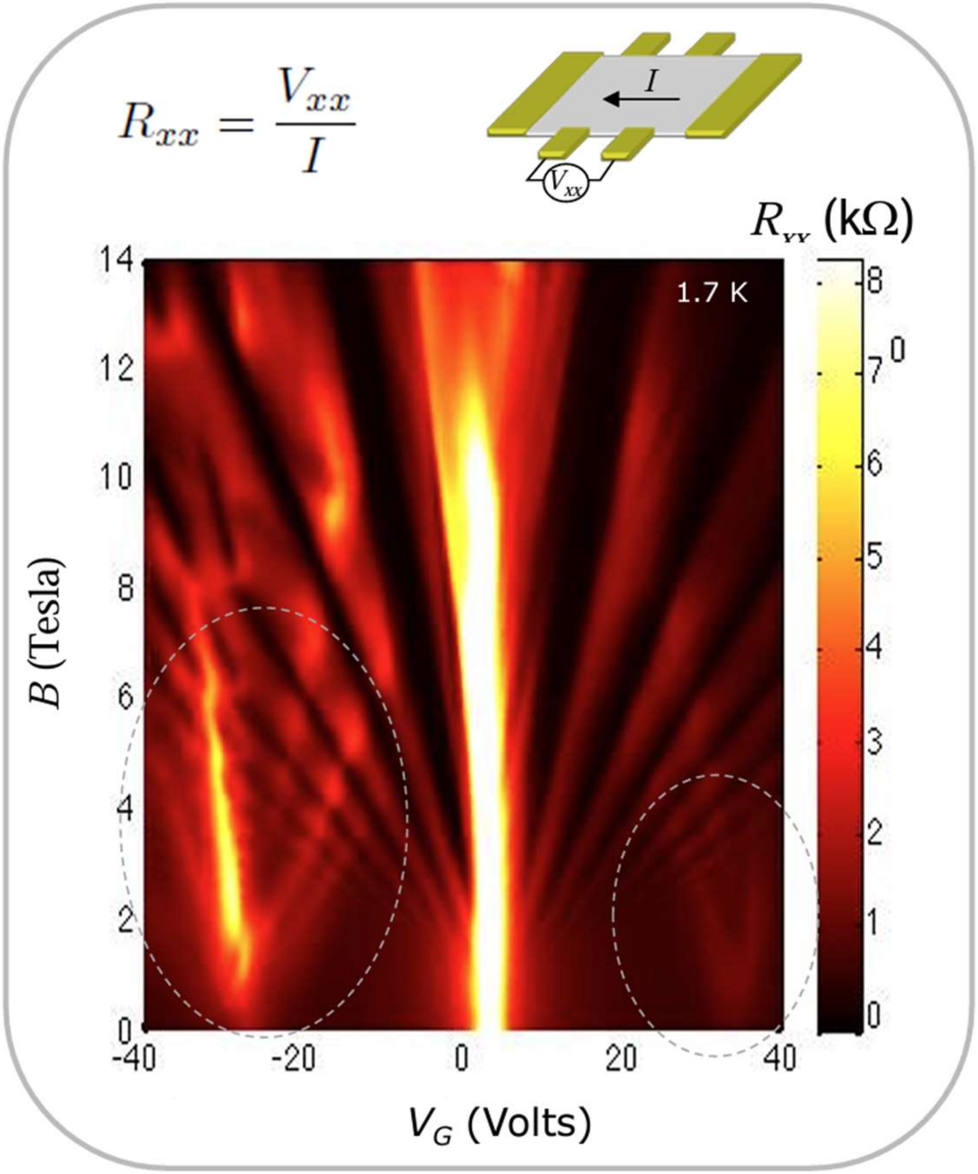

$$(R_{xy}^Q)^{-1} = \sigma_{xy}^Q = \frac{e^2}{h}\nu$$

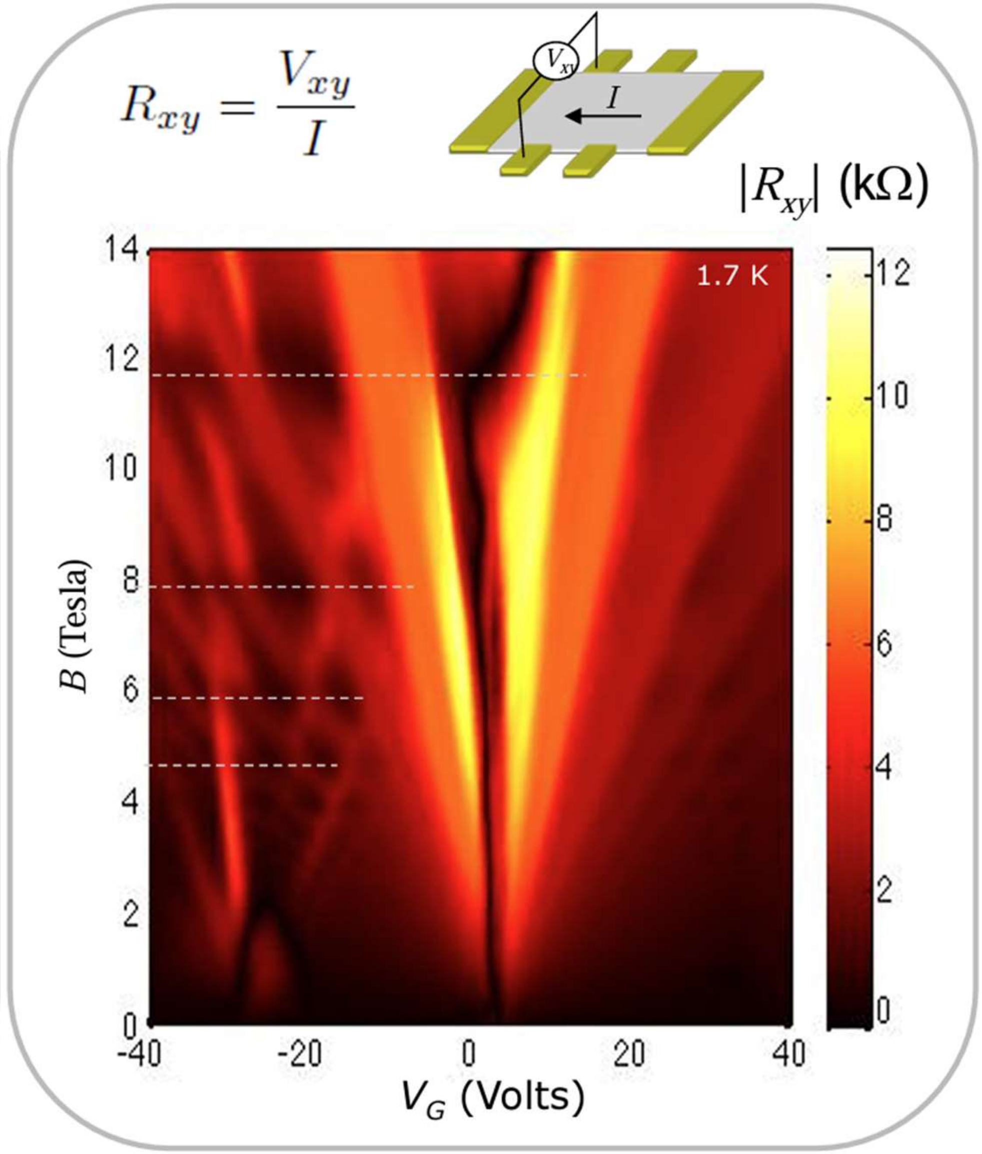


# Abnormal QHE in graphene/hBN

Special Samples with Large Moire Unit Cell

Low Magnetic field regime

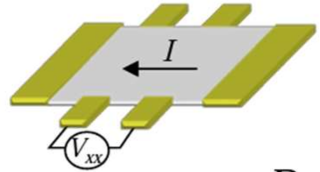


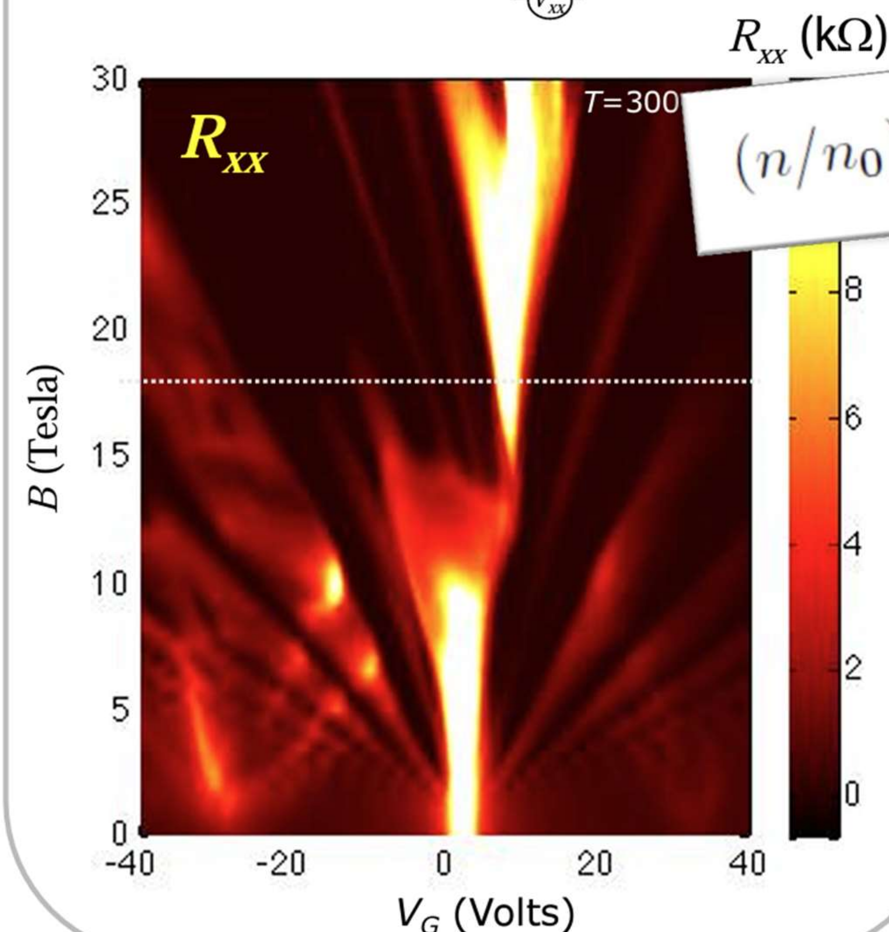



# Evidence of Hofstadters butterfly

## Quantum Hall-like Transport

$$R_{xx} = \frac{V_{xx}}{I}$$



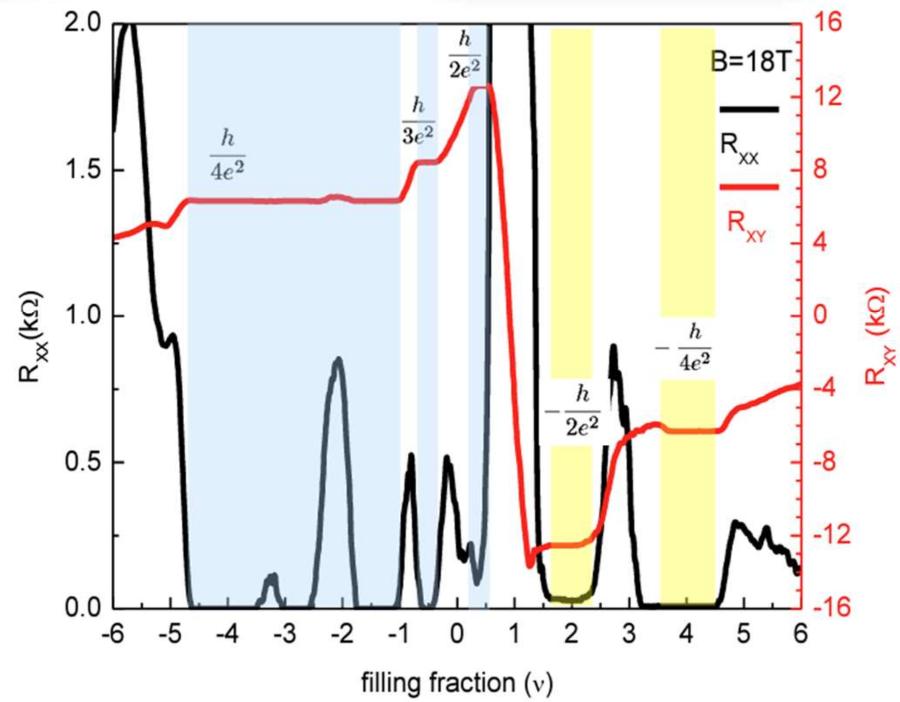




Landau level filling factor $\nu = \frac{\phi_0}{B} n$

Quantum Hall conductance $R_{xy}^{-1} = \frac{e^2}{h} t$

$$(n/n_0) = t(\phi/\phi_0) + s$$

~~$\nu = t$~~ $\in \mathbb{Z}$



# Few years later