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Spring College on Computational Nanoscience

17 - 28 May 2010

Electric Transport in Carbon Nanotubes and Graphene

Philip KIM

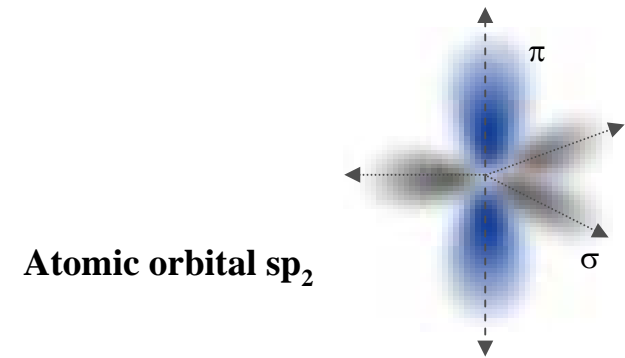
*Dept. of Physics, Columbia University
New York
U.S.A.*



Electric Transport in Nanotubes and Graphene

Philip Kim
Department of Physics
Columbia University

SP₂ Carbon: 0-Dimension to 3-Dimension



0D

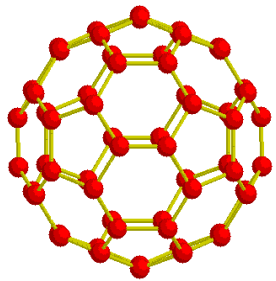
1D

2D

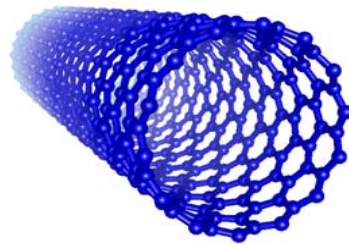
3D



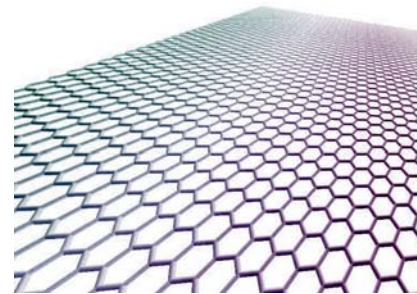
Fullerenes (C₆₀)



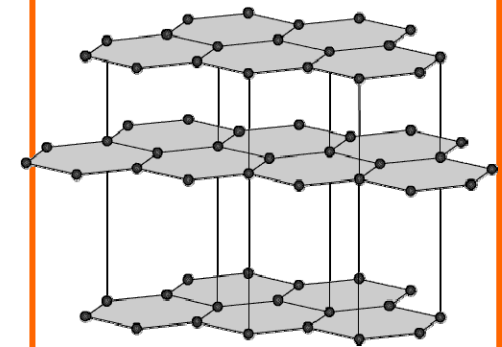
Carbon Nanotubes



Graphene

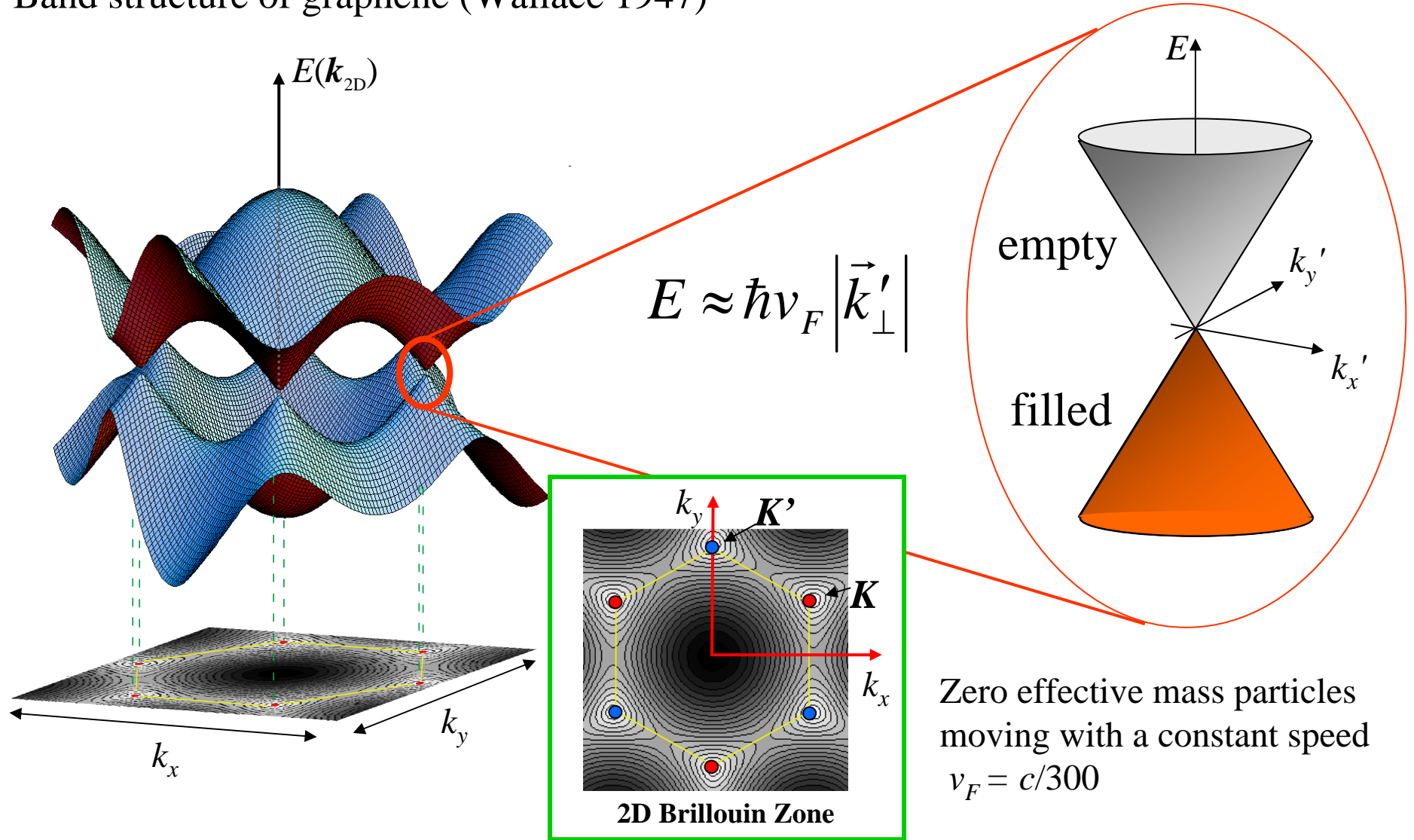


Graphite



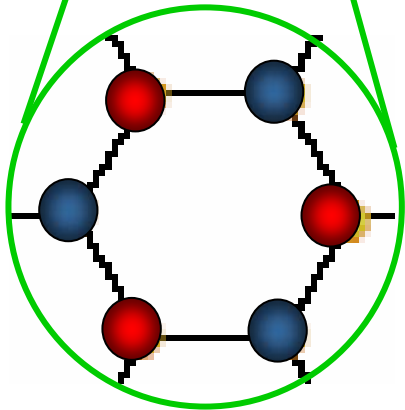
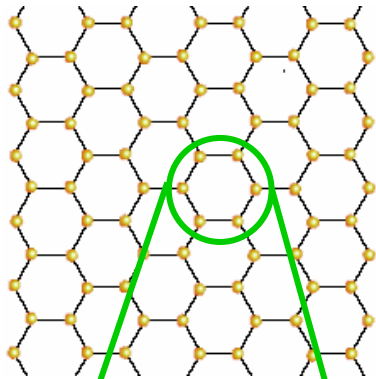
Electronic Band Structure of Graphene

Band structure of graphene (Wallace 1947)



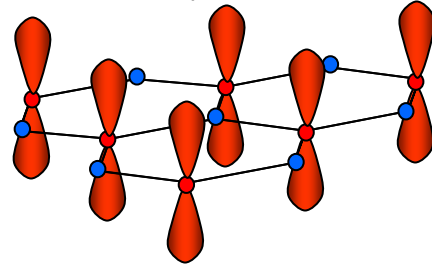
Graphene Lattice Symmetry: Pseudo Spinor

Graphene Lattice Structures



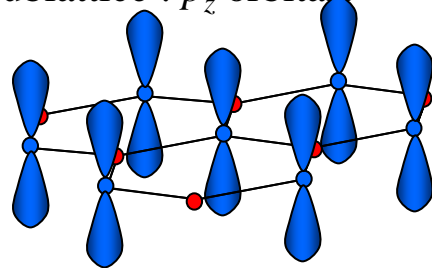
Two inequivalent lattice sites!

'A' sublattice: p_z orbitals



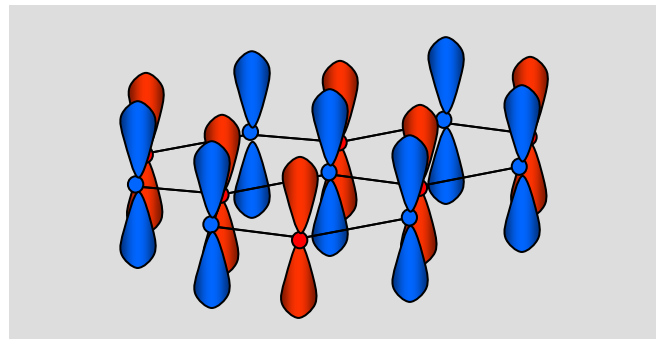
$|A\rangle$

'B' sublattice: p_z orbitals

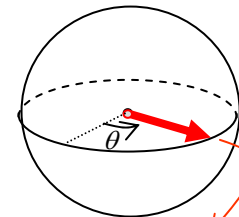
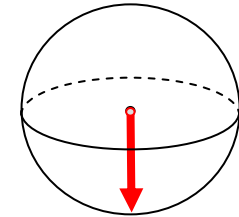
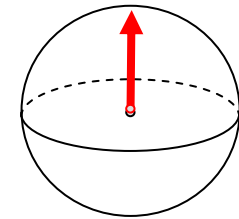


$|B\rangle$

Superposition: $|A\rangle + e^{i\theta} |B\rangle$

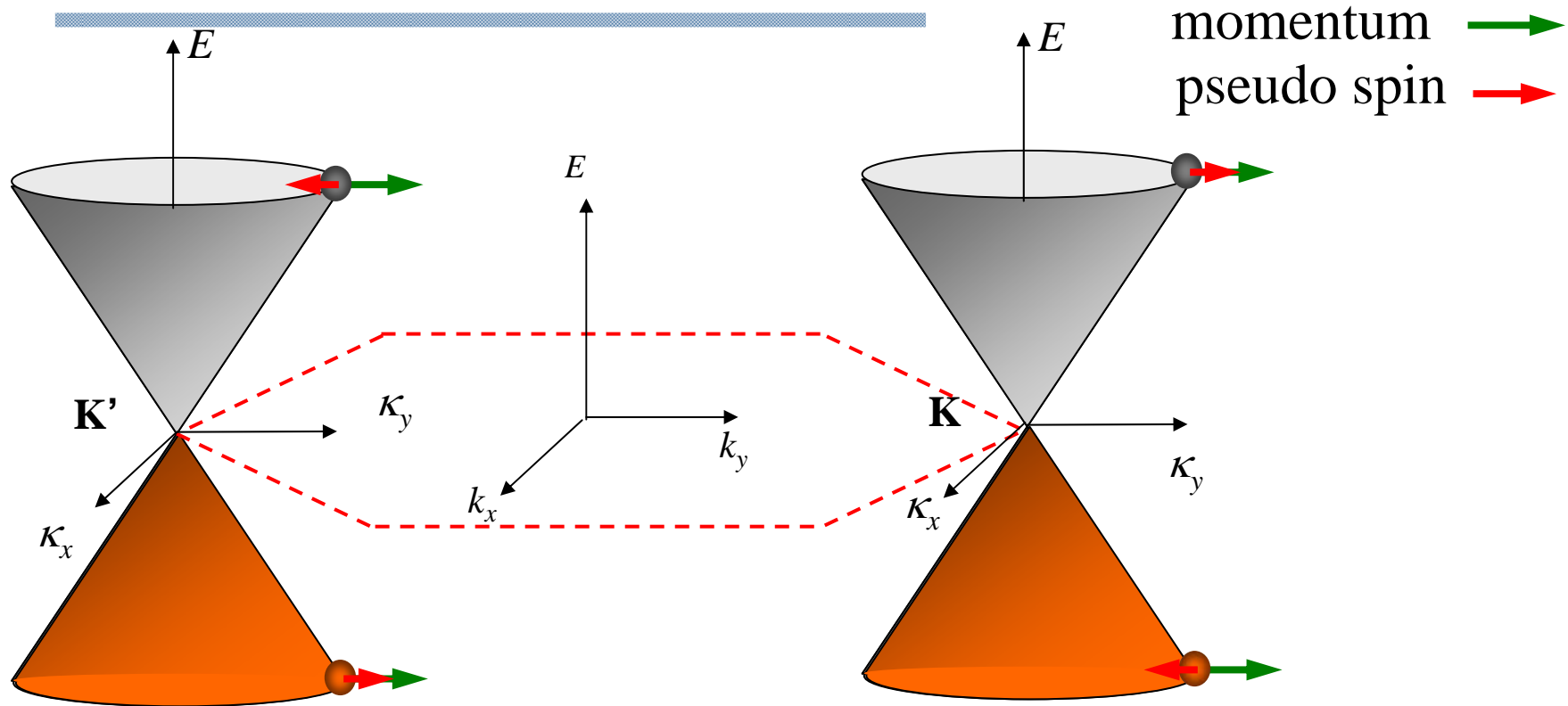


Spinor Representation



Pseudo spin

Dirac Fermions in Graphene : “Helicity”



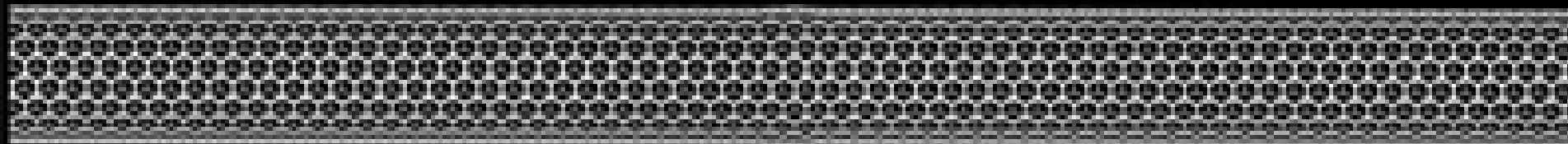
Effective Dirac Equations

$$H_{eff} = \pm \hbar v_F \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} = \pm \hbar v_F \vec{\sigma} \cdot \vec{k}_\perp$$

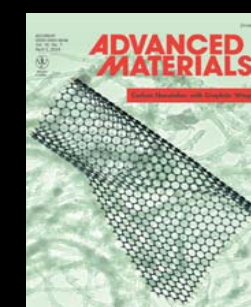
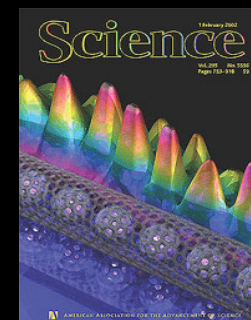
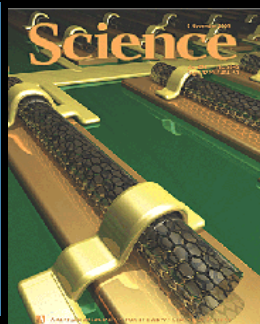
$$|k_\perp\rangle = e^{ik \cdot r} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta_k} \end{pmatrix}$$

$$\theta_k = \tan^{-1}(k_y / k_x)$$

Single Wall Carbon Nanotube



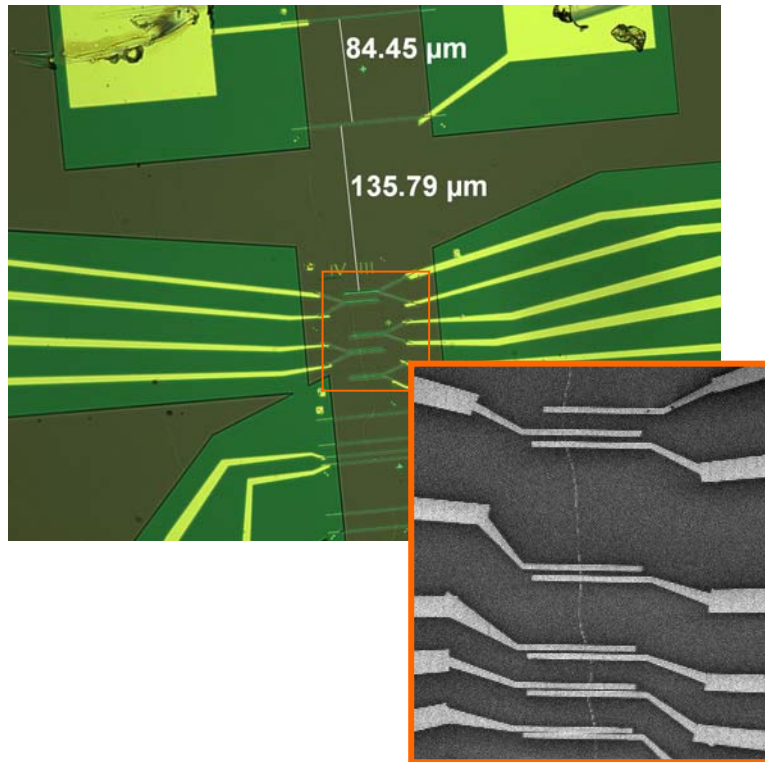
.... since 1991



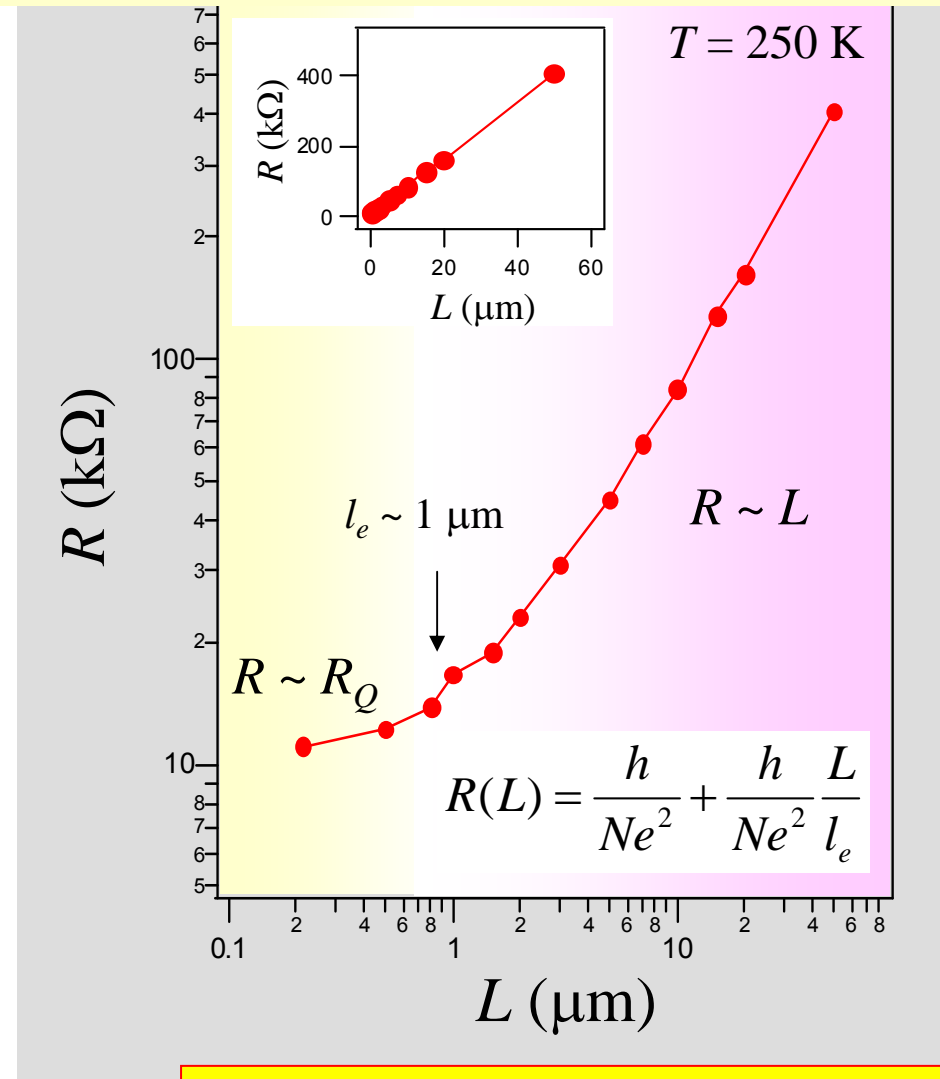
Extremely Long Mean Free Path in Nanotubes

See also S. Frank, P. Poncharal, Z. L. Wang, and W. A. de Heer, *Science* **280**, 1744-1746 (1998)

Multi-terminal Device with Pd contact



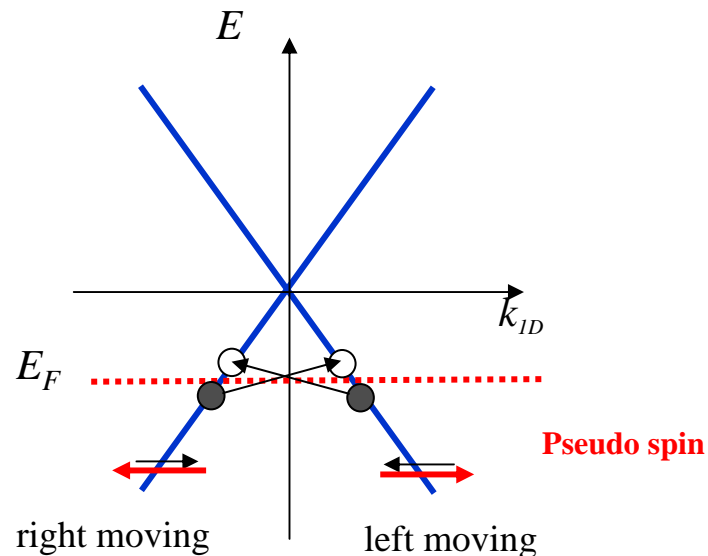
* Scaling behavior of resistance:
 $R(L)$



Room temperature mean free path > 0.5 μm

Extremely Long Mean Free Path of Nanotubes: Role of Pseudo Spin

1D band structure of nanotubes



$$\frac{1}{\tau} = \frac{2\pi}{\hbar} \left\langle \vec{k}' \sigma'_{pseudo} \left| V(\vec{r}) \right| \vec{k} \sigma_{pseudo} \right\rangle$$

- Small momentum transfer backward scattering becomes inefficient since it requires pseudo spin flipping.

Journal of the Physical Society of Japan
Vol. 67, No. 8, August, 1998, pp. 2857-2862

Berry's Phase and Absence of Back Scattering in Carbon Nanotubes

Tsuneya ANDO, Takeshi NAKANISHI,¹ and Rūichiro SAITO²

*Institute for Solid State Physics, University of Tokyo
7-22-1 Minato-ku, Roppongi, Tokyo 106*

¹ *The Institute of Physical and Chemical Research (RIKEN)
2-1 Hirosawa, Wako-shi, Saitama 351-01*

² *Department of Electronics Engineering
University of Electro-Communications, Chofugaoka, Chofu, Tokyo 182*

(Received March 16, 1998)

The absence of back scattering in carbon nanotubes is shown to be ascribed to Berry's phase which corresponds to a sign change of the wave function under a spin rotation of a neutrino-like particle in a two-dimensional graphite. Effects of trigonal warping of the bands appearing in a higher order $\mathbf{k}\cdot\mathbf{p}$ approximation are shown to give rise to a small probability of back scattering.

VOLUME 83, NUMBER 24

PHYSICAL REVIEW LETTERS

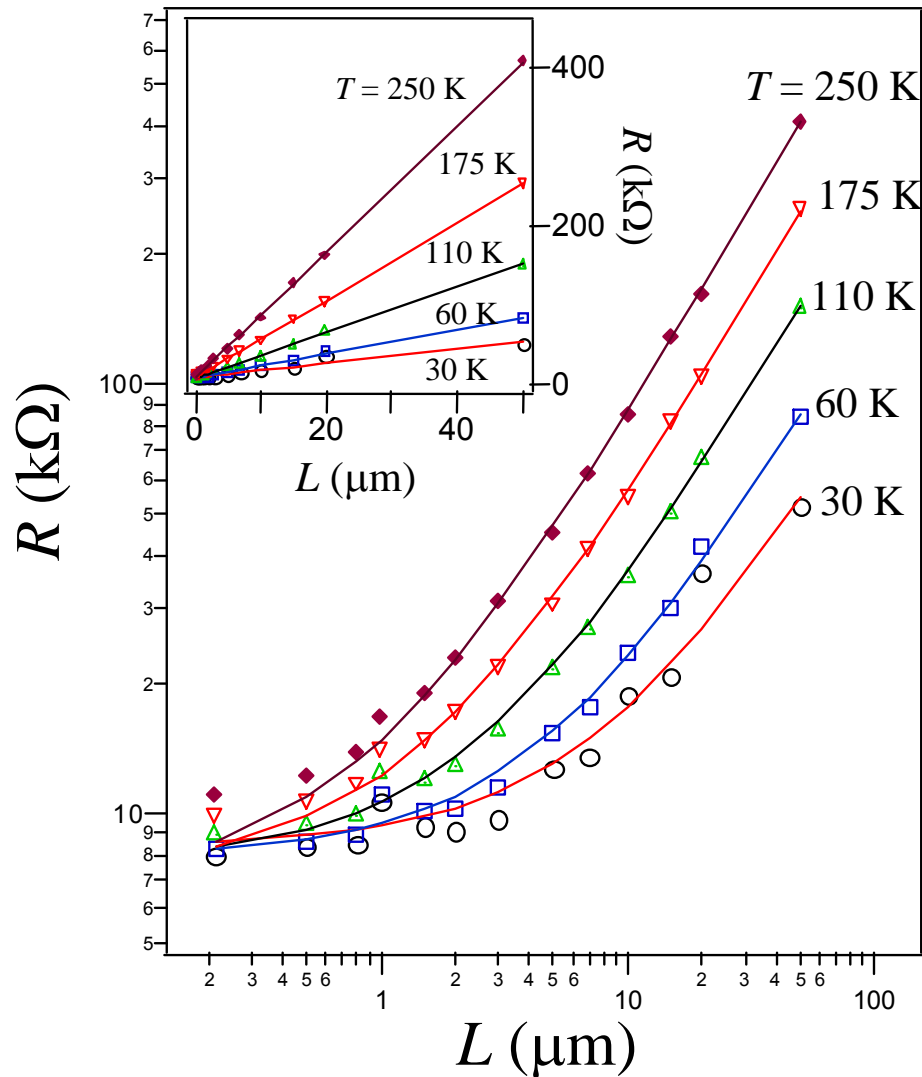
13 DECEMBER 1999

Disorder, Pseudospins, and Backscattering in Carbon Nanotubes

Paul L. McEuen, Marc Bockrath, David H. Cobden,* Young-Gui Yoon, and Steven G. Louie
*Department of Physics, University of California, and Materials Science Division, Lawrence Berkeley National Laboratory,
Berkeley, California 94720*
(Received 7 June 1999)

We address the effects of disorder on the conducting properties of metal and semiconducting carbon nanotubes. Experimentally, the mean free path is found to be much larger in metallic tubes than in doped semiconducting tubes. We show that this result can be understood theoretically if the disorder potential is long ranged. The effects of a pseudospin index that describes the internal sublattice structure of the states lead to a suppression of scattering in metallic tubes, but not in semiconducting tubes. This conclusion is supported by tight-binding calculations.

Electron Mean Free Path of Nanotube

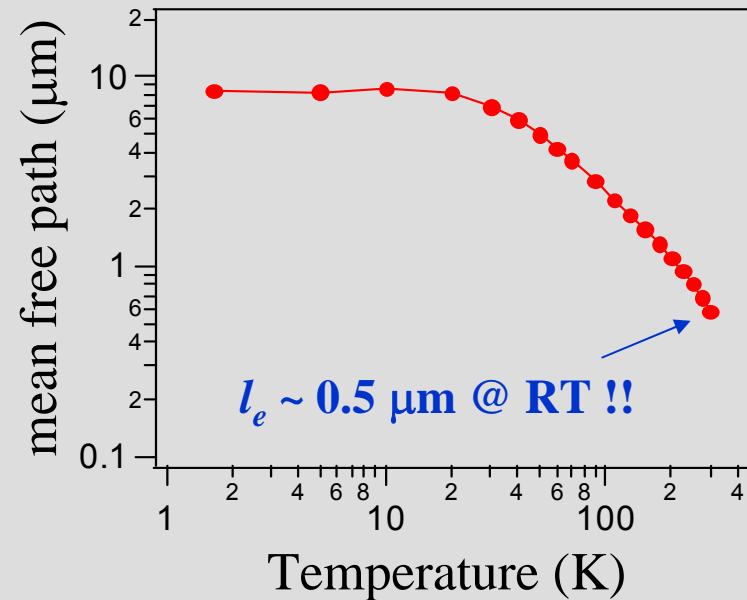


Lines are fit to

$$R(L) = R_c + \frac{h}{4e^2} + \frac{h}{4e^2} \frac{L}{l_e}$$

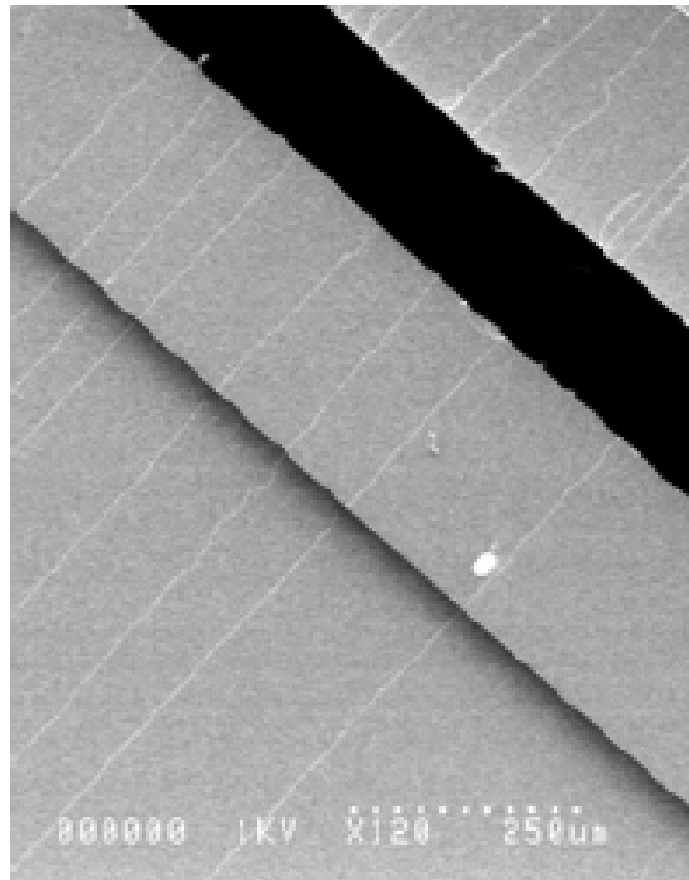
$$\frac{h}{4e^2} = 6.45 \text{ k}\Omega$$

Non-ideal contact resistance $R_c < 2 \text{ k}\Omega$

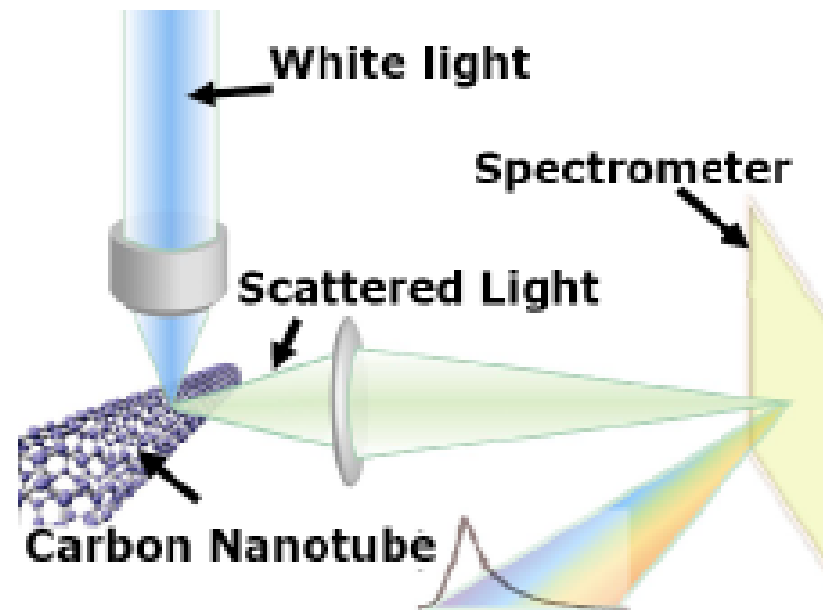


Characterization of Nanotube Structures by Rayleigh Light Scattering

Nanotube Growth over trenches



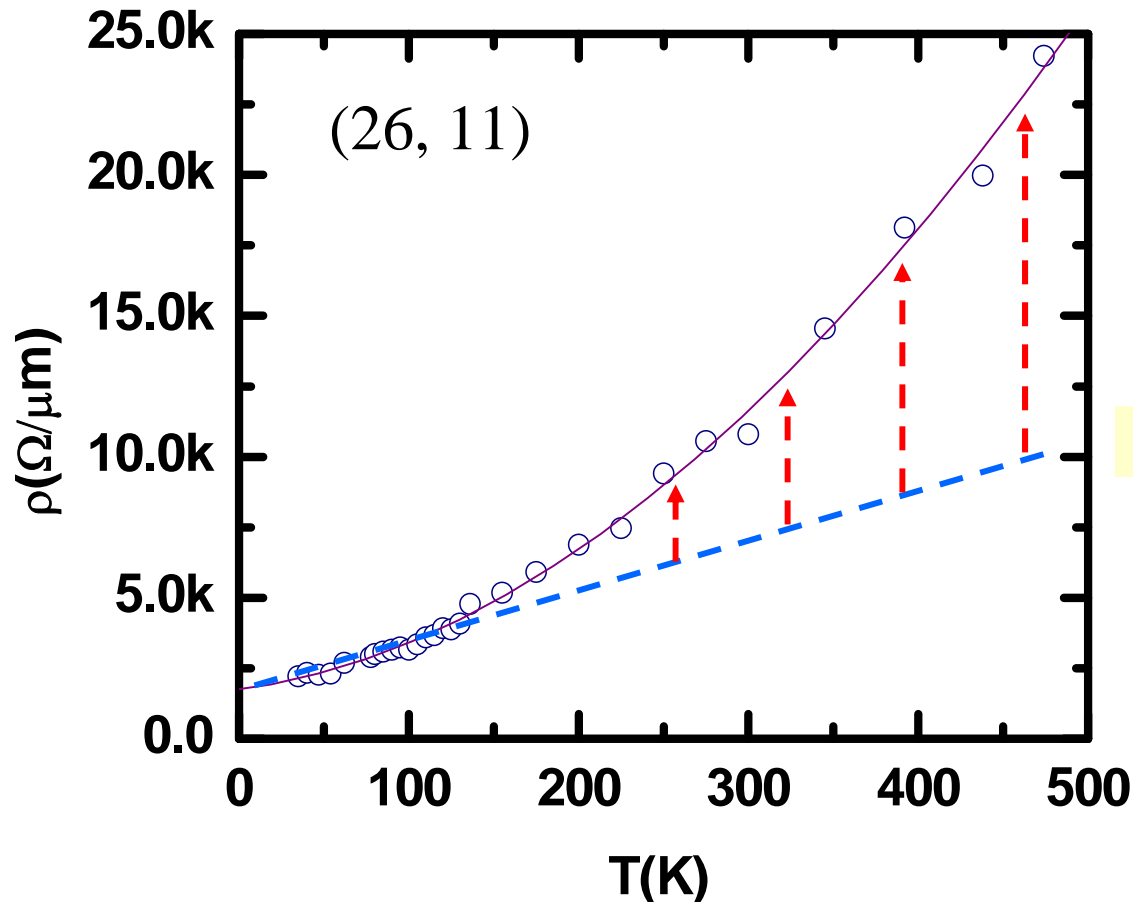
Rayleigh Scattering Characterization



Brus, Heinz, Hone, O'Brien groups, Science 306,1540 (2004)

Temperature Dependent Resistivity

B. Chandra M. Purewal, P. Kim and J. Hone



Super linear behaviors
for $T > 150$ K

Scattering due to acoustic phonons

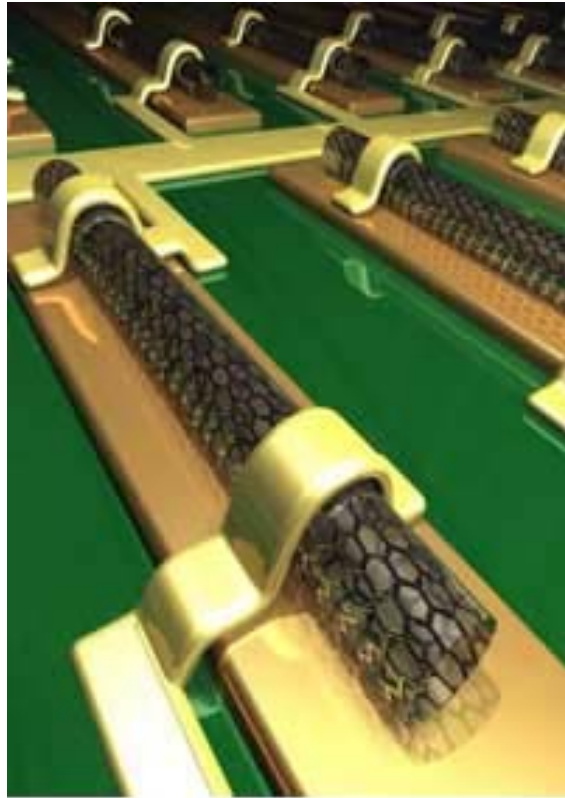
$$\frac{1}{\tau_{ac}} = 2 \frac{2\pi}{\hbar} \Xi^2 \left(\frac{k_B T}{2\rho v_s^2} \right) \frac{1}{\hbar v_F}$$

Enhanced scattering activated $T > 150$ K

Carbon Electronics: Challenges

Pros:

- High mobility
- High on-off ratio (nanotubes)
- High critical current density

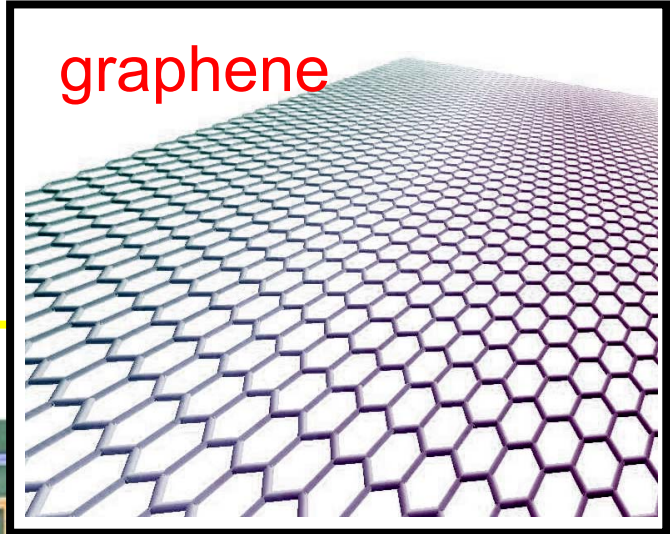


Artistic dream (DELFT)

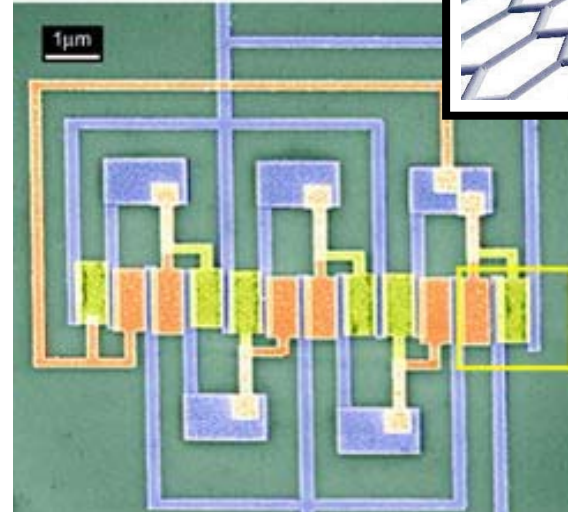
Con:

- Controlled growth

graphene



IBM, Avouris group



Nanotube Ring Oscillators

Graphene Sample Preparation

SCIENTIFIC AMERICAN.COM

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March 20, 2008

D.I.Y. Graphene: How to Make One-Atom-Thick Carbon Layers With Sticky Tape

Graphene, science's latest wonder material, is surprisingly easy to produce. JR Minkel explores how to make the novel substance, which is discussed in detail in [Carbon Wonderland](#)

By JR Minkel



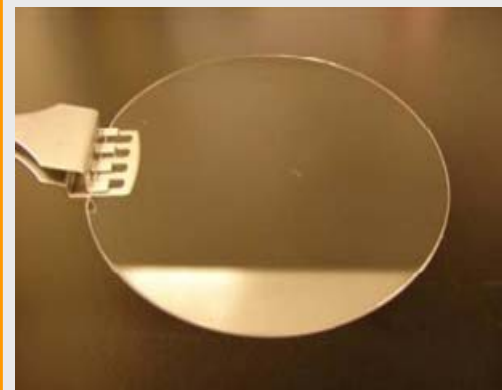
Pablo Janillo-Herrero [ENLARGE IMAGE](#)



| Slide 1 of 9

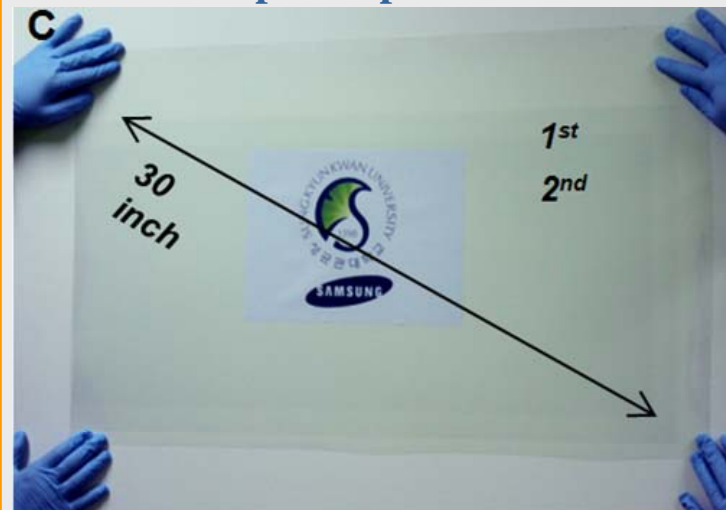
Work in a relatively clean environment (or even a clean room, if possible); stray dirt or hair wreaks havoc with graphene samples. To get that clean room vibe on the cheap, grab some goggles and rubber gloves, along with a shower cap for your head as well as two more for each foot.

Epitaxial graphene on SiC



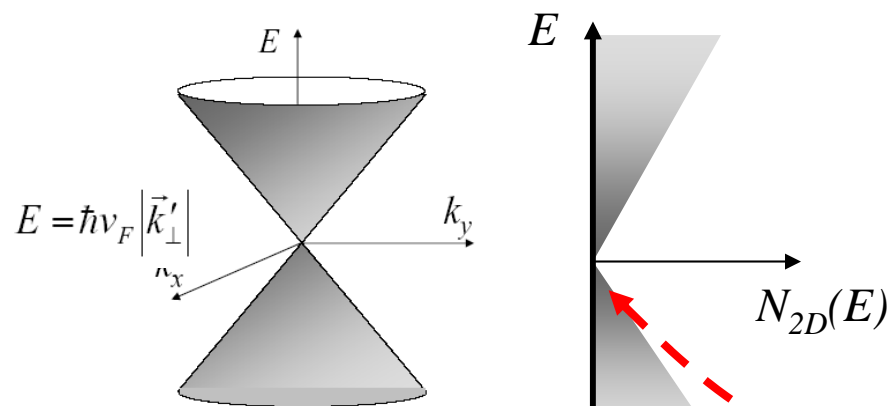
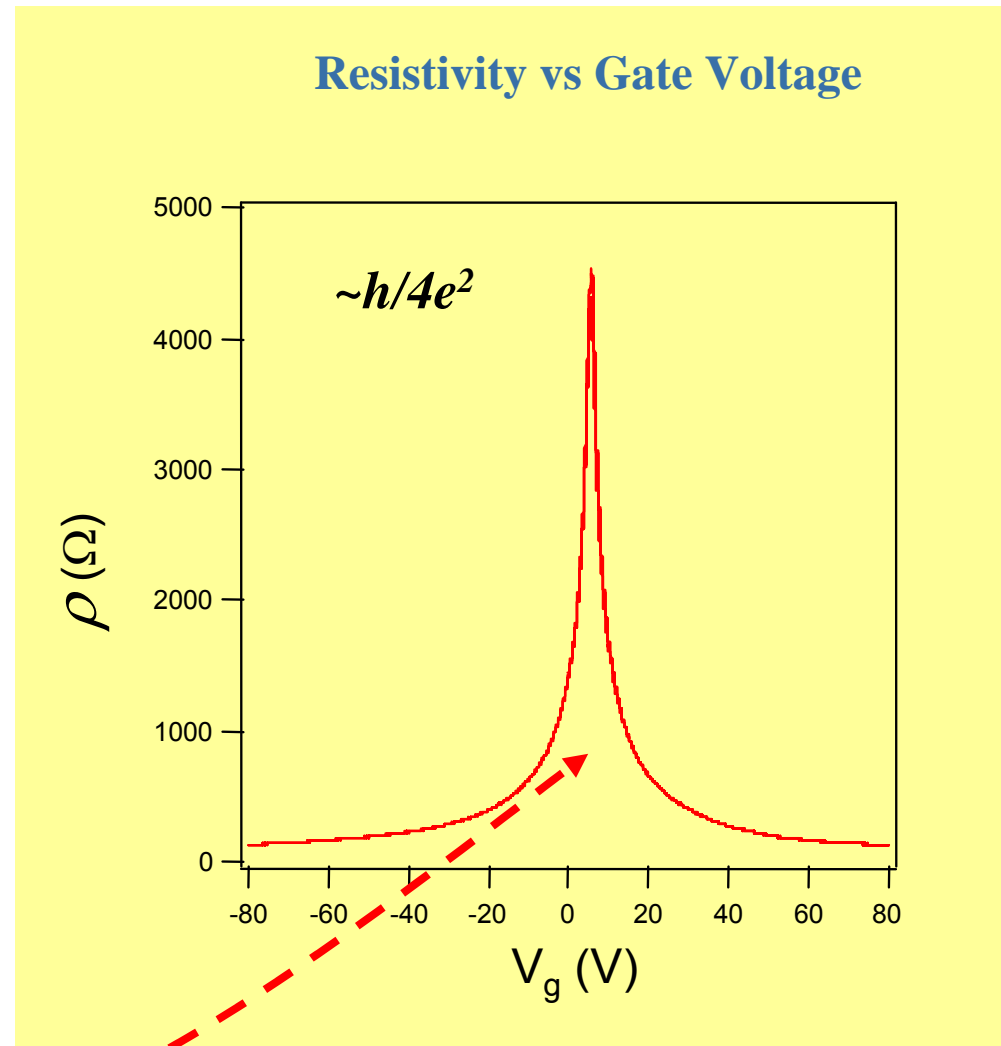
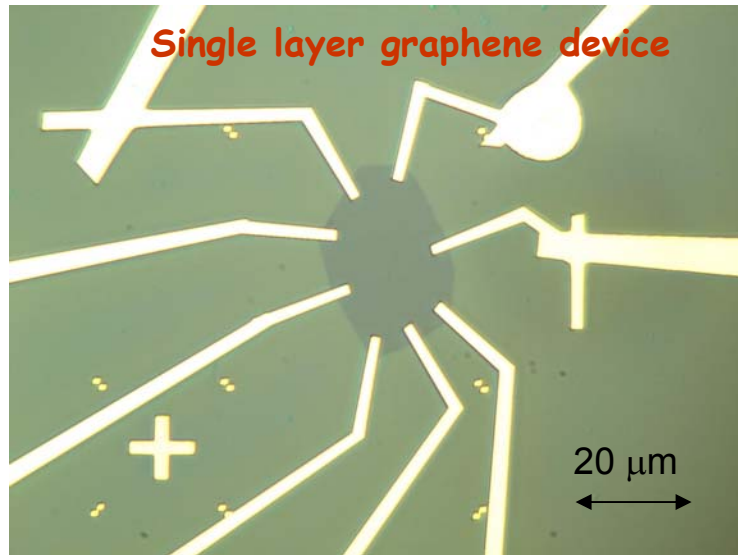
GTech, IBM, NRL, HRL, Purdue, ...

Chemical Vapor Deposition



SKKU, MIT, Austin, ...

Field Effective Transport in Single Layer Graphene

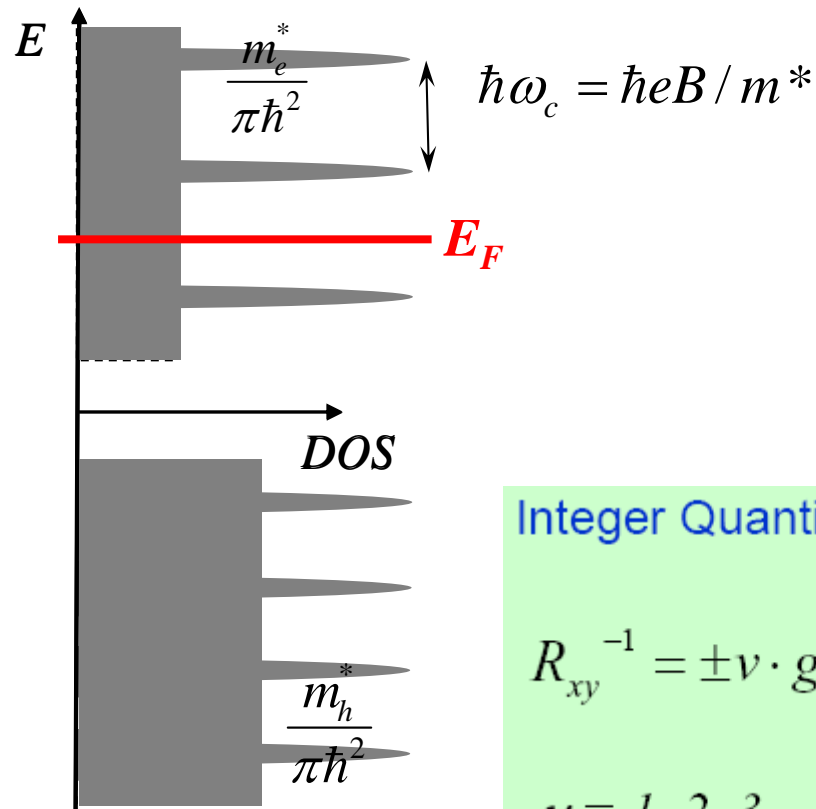


$$\rho^{-1} = e^2 v_F l_e N_{2D}$$

2D Gas in Quantum Limit : Conventional Case

Density of States

Landau Levels in Magnetic Field



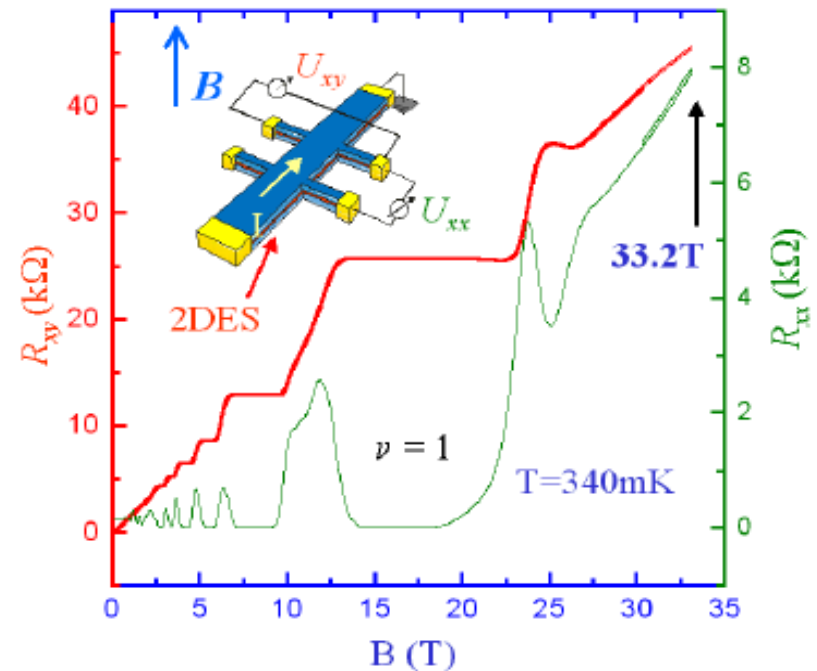
Integer Quantization:

$$R_{xy}^{-1} = \pm \nu \cdot g_s \cdot \frac{e^2}{h}$$

$$\nu = 1, 2, 3 \dots$$

$$g_s = 2 \text{ (spin)}$$

Quantum Hall Effect in GaAs 2DEG

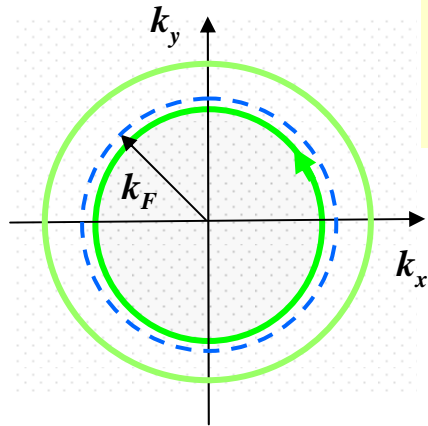


Graphene

- Vanishing carrier mass near Dirac point
- Strict electron hole symmetry
- Electron hole degeneracy $\omega_c = \frac{eB}{m^*}$

Berry's Phase and Magneto Oscillations

Landau orbit near the Fermi level



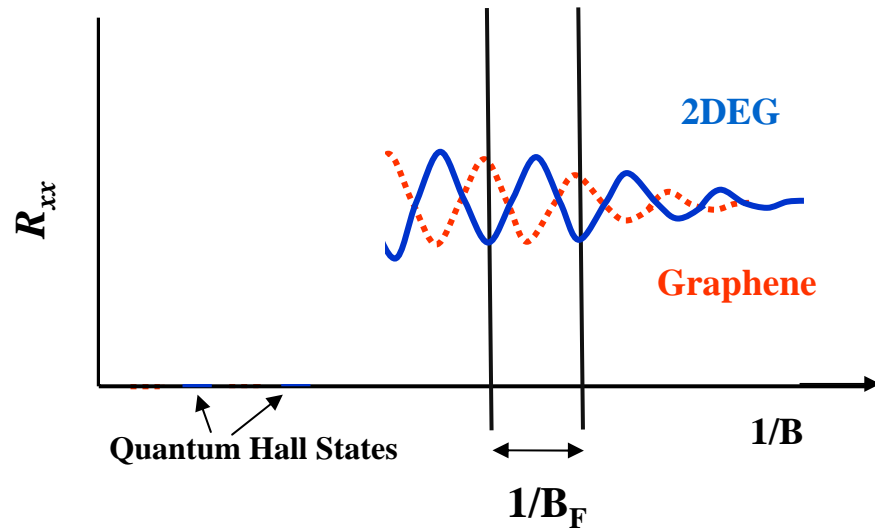
Magnetic flux in cyclotron orbit

$$\Phi_B = \Phi_0 B_F/B$$

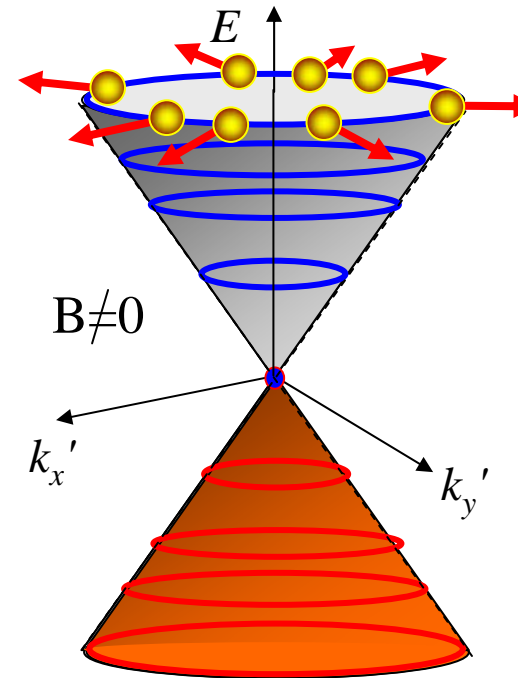
$$\Phi_0 = h/e$$

$$B_F = \Phi_0 k_F^2 / 4\pi$$

$$\psi \sim \psi_0 \exp[2\pi(\Phi_B/\Phi_0)]$$



Graphene: $H_{eff} = \hbar v_F \vec{\sigma} \cdot \vec{k}'_{\perp}$



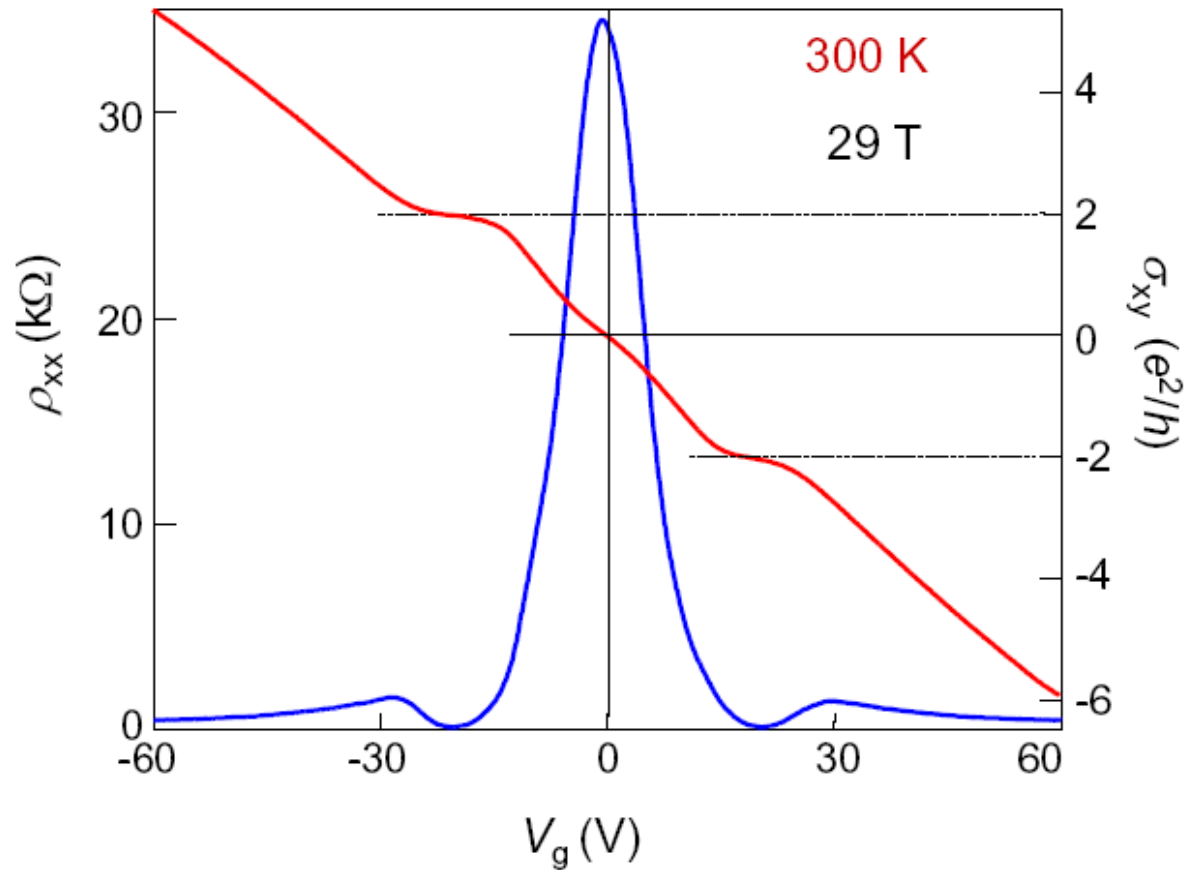
Pseudo Spin

$$S = \hbar/2$$

$$\theta = 2\pi$$

$$\psi \sim \psi_0 \exp[2\pi(\Phi_B/\Phi_0) - \underbrace{S\theta/\hbar}_{\pi}]$$

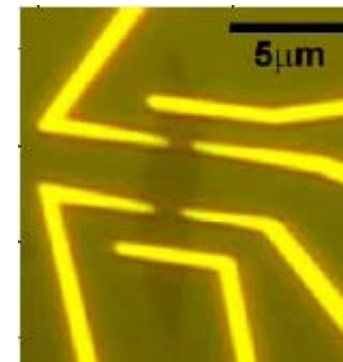
Room Temperature Quantum Hall Effect



$$E_n = \pm \sqrt{2e\hbar v_F^2 |n| B}$$

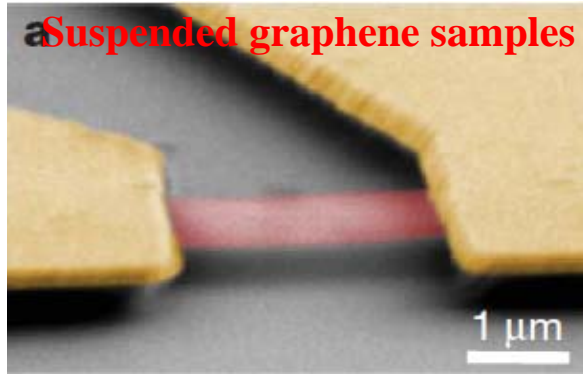
$$E_1 \sim 100 \text{ meV @ } 5 \text{ T}$$

Typical sample on SiO₂
mobility: $\sim 15,000 \text{ cm}^2/\text{Vsec}$

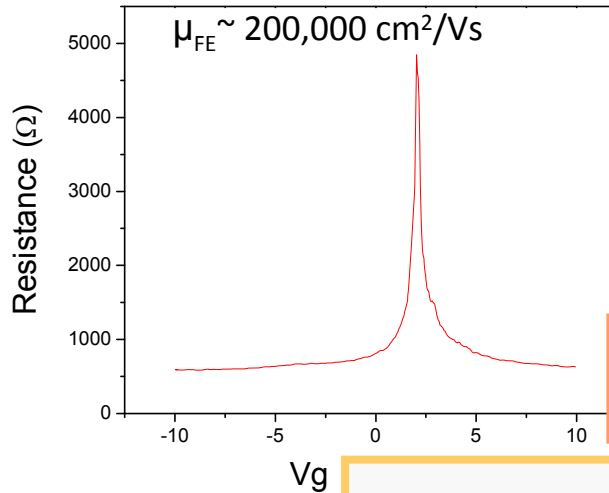


Novoselov, Jiang, Kim and Geim et al. *Science* (2007)

Quantum Hall Effect in Suspended Graphene

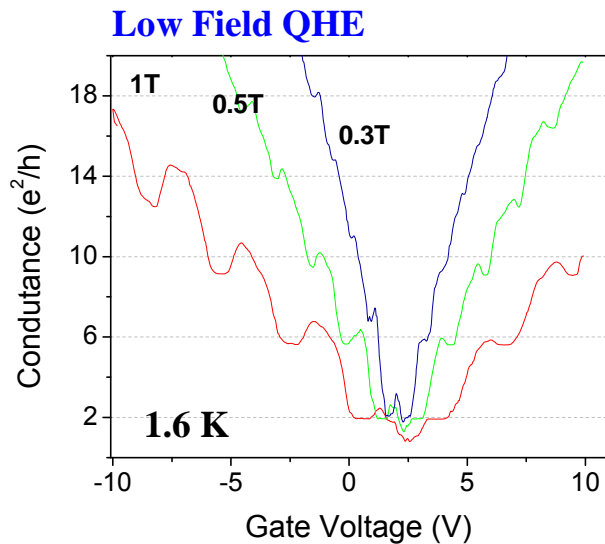


Bolotin et al., (2008); Du et al., (2008)

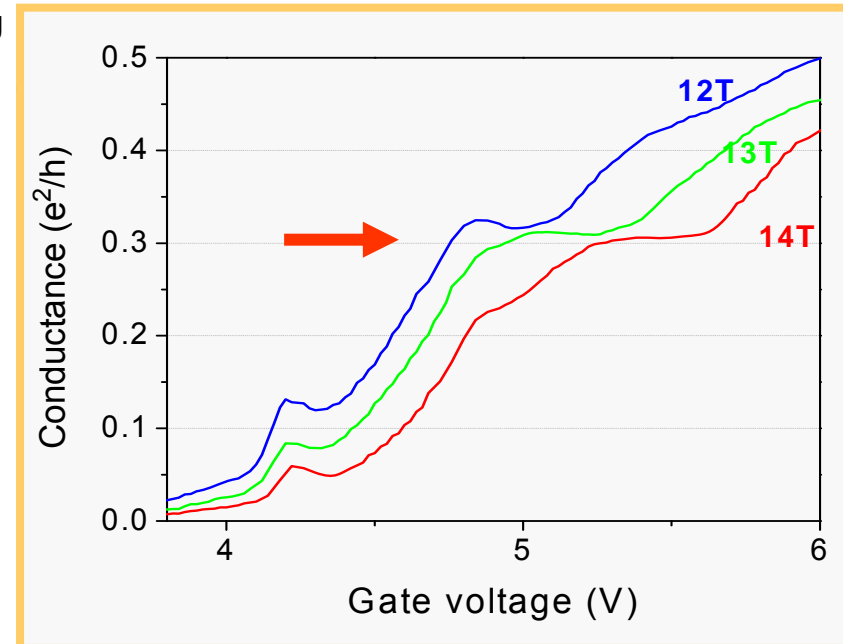


- Cleaning: current annealing
Bachtold et al. (2007)
- Mechanical stability
J. Lau et al. (2009)

$\nu=1/3$ FQHE is observed!!

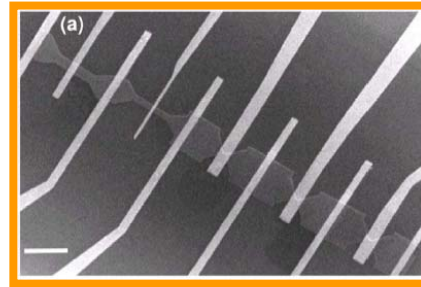


Increasing B

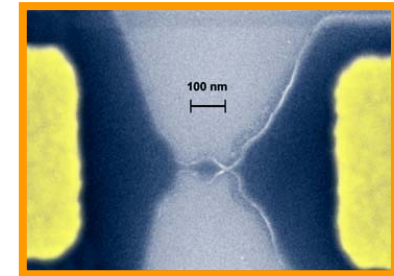


Creation of Energy Gap in Graphene

- Confinement of Dirac Particles: **Nanoribbons, Quantum Dot**



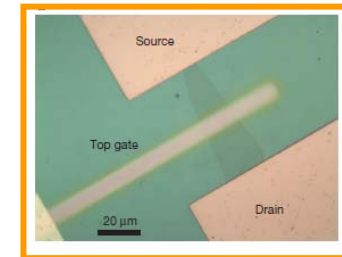
(Columbia, IBM, ...)



(Manchester, ETH, ...)

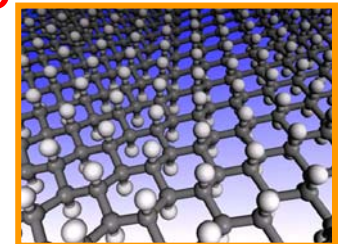
-
- Breaking Symmetry: **Biased Bilayer Graphene**

(Manchester, DELFT, Berkeley, Columbia, ...)

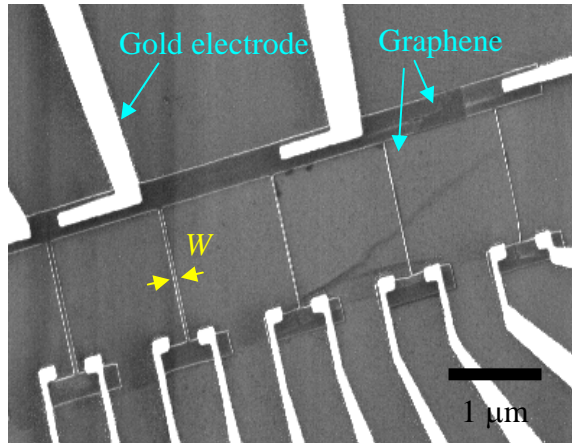


-
- Chemical Treatment: **Graphane, Graphene Oxide**

(Manchester, Rutgers, ...)

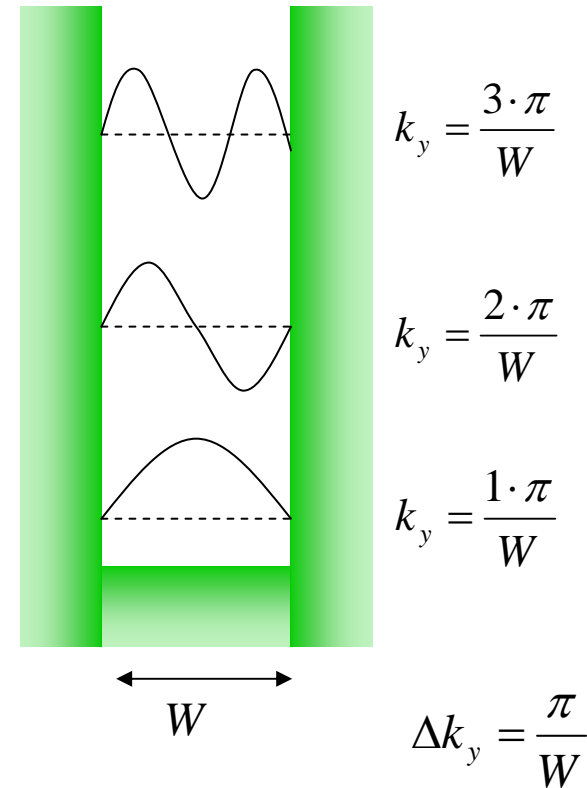
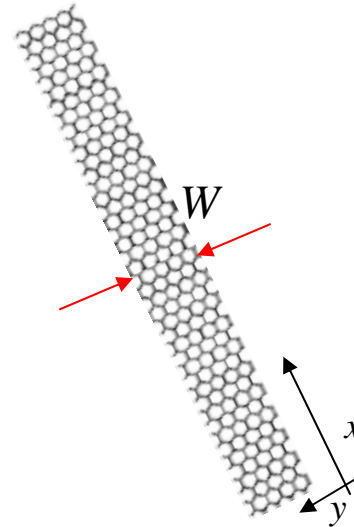


Graphene Nanoribbons: Confined Dirac Particles



$10 \text{ nm} < W < 100 \text{ nm}$

Dirac Particle Confinement



$$E = \pm \hbar v_F \sqrt{k_x^2 + (\pi n / W)^2}$$

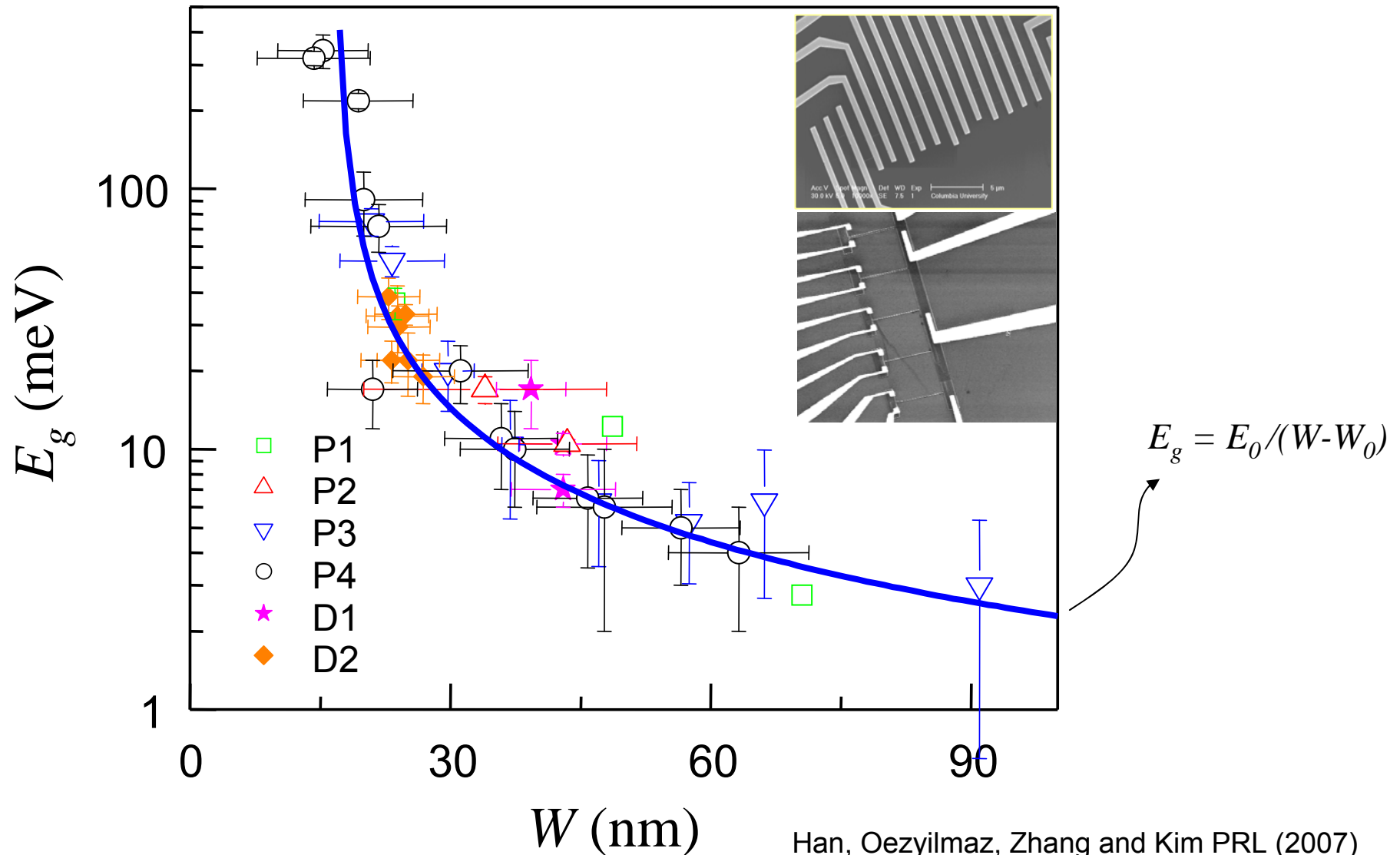
$$E_{\text{gap}} \sim \hbar v_F \Delta k \sim \hbar v_F / W$$

Graphene nanoribbon theory partial list

- K. Nakada, M. Fujita, G. Dresselhaus, M. S. Dresselhaus, Phys. Rev. B **54**, 17954 (1996).
- K. Wakabayashi, M. Fujita, H. Ajiki, M. Sigrist, Phys. Rev. B **59**, 8271 (1999).
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- D. A. Areshkin, D. Gunlycke, C. T. White, Nano Lett. **7**, 204 (2007).

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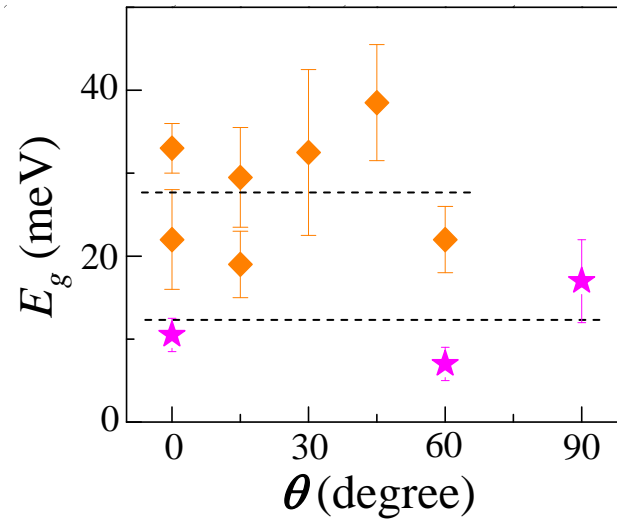
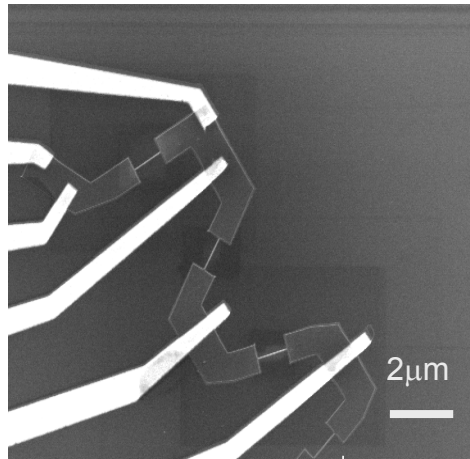
Scaling of Energy Gaps in Graphene Nanoribbons



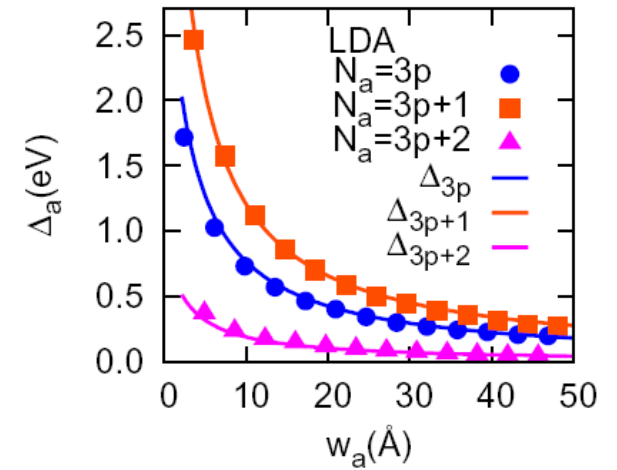
Han, Oezylmaz, Zhang and Kim PRL (2007)
Chen, Lin, Rooks, and Avouris, Physica E. (2007)

Graphene Nanoribbons Edge Effect

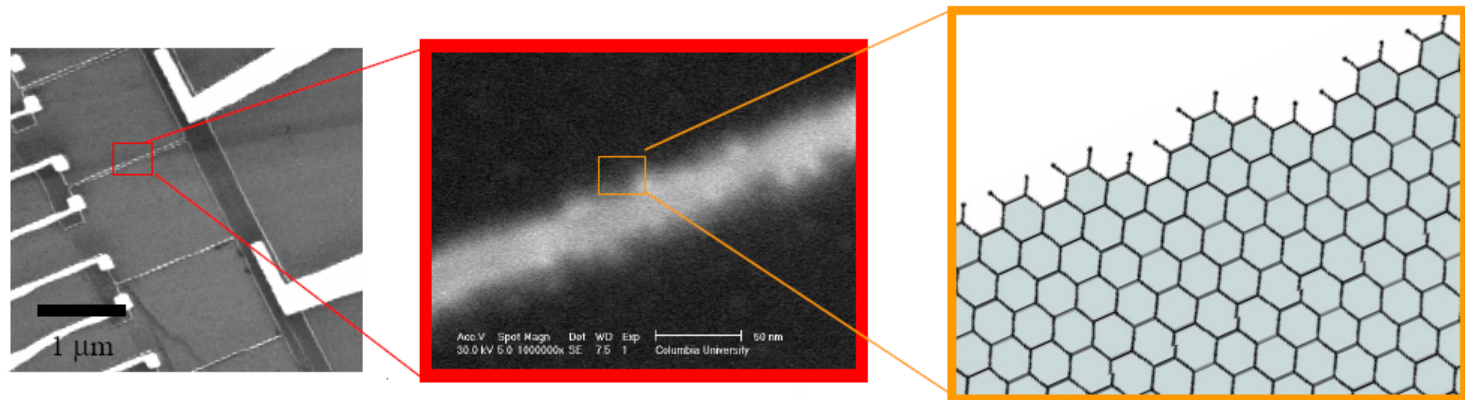
Crystallographic Directional Dependence



Son, et al, PRL. 97, 216803 (2006)

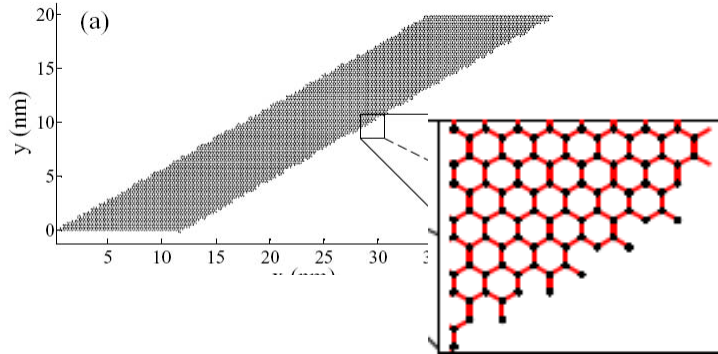


Rough Graphene Edge Structures



Localization of Edge Disordered Graphene Nanoribbons

Querlioz et al., Appl. Phys. Lett. **92**, 042108 (2008)

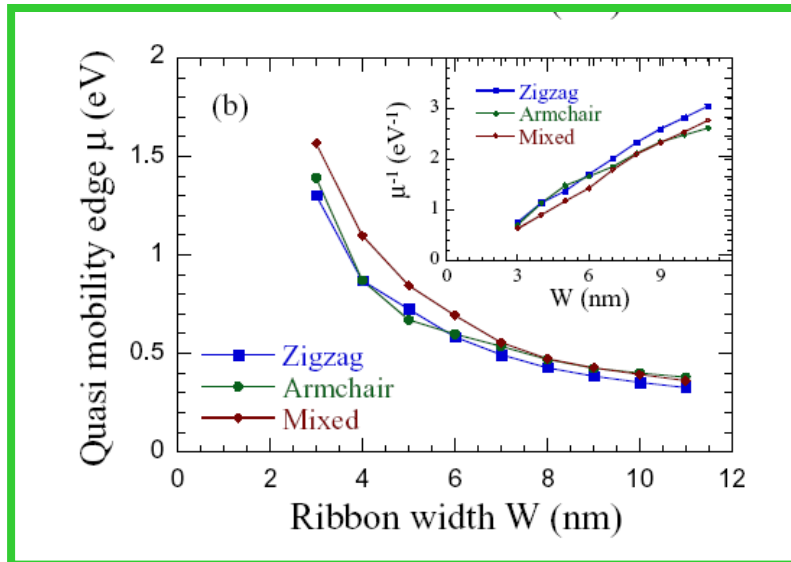
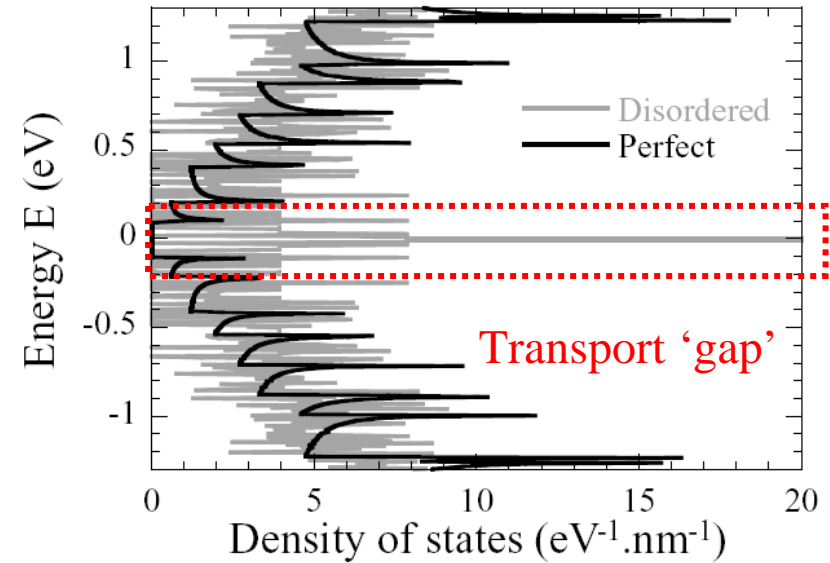


See also:

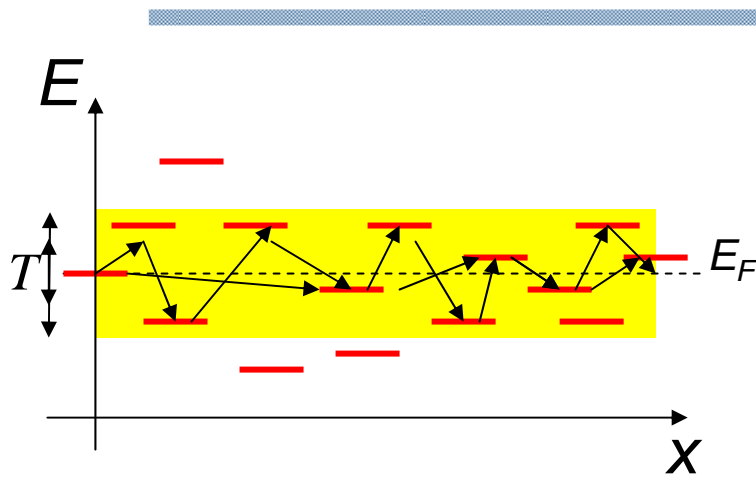
Gunlycke et al, Appl. Phys. Lett. **90** (14), 142104 (2007).

Areshkin et al, Nano Lett. **7** (1), 204 (2007)

Lherbier et al, PRL 100 036803 (2008)

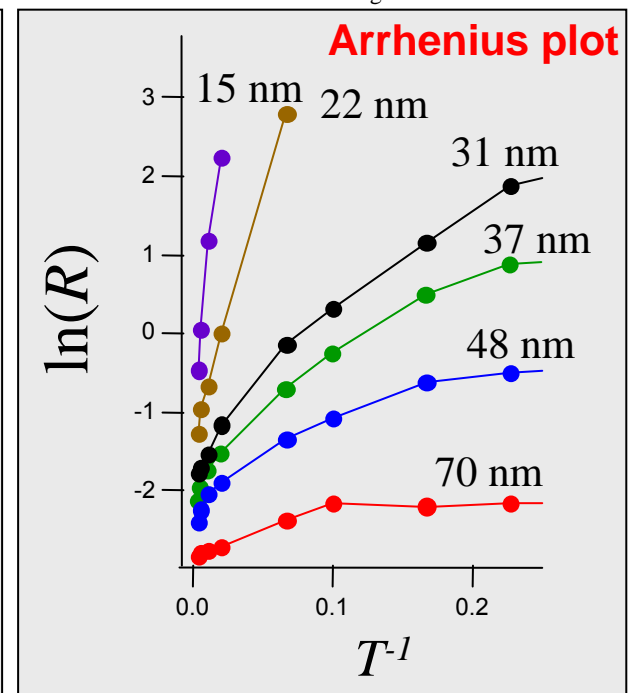
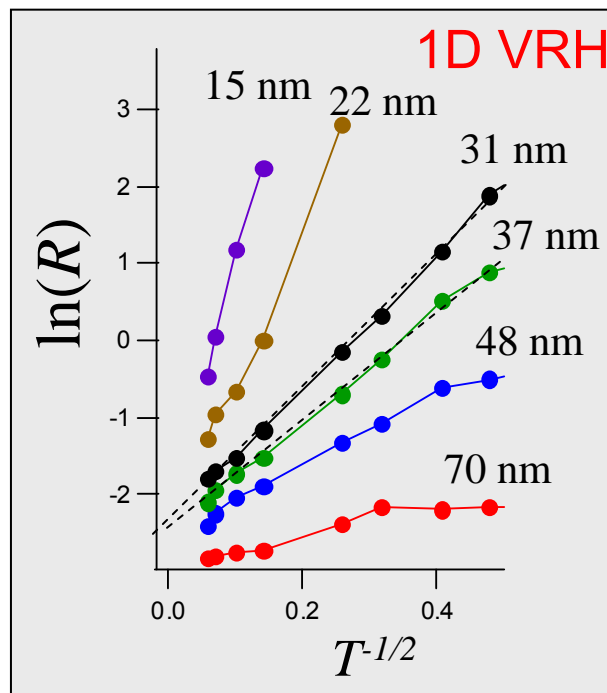
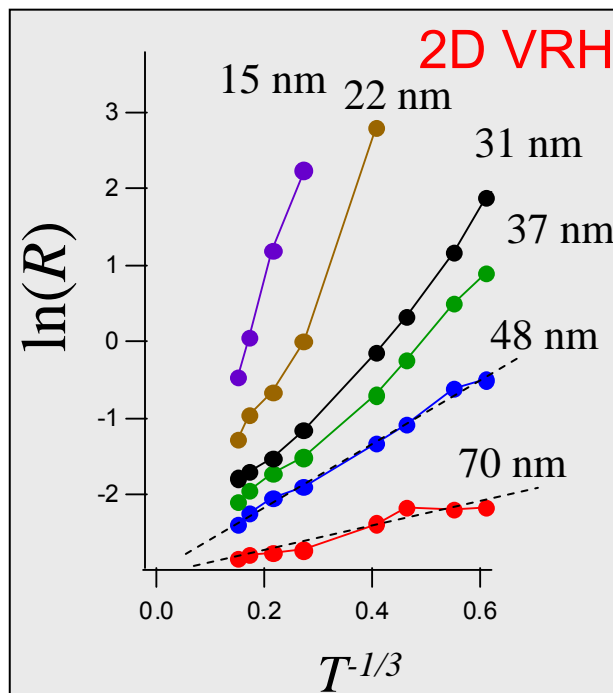
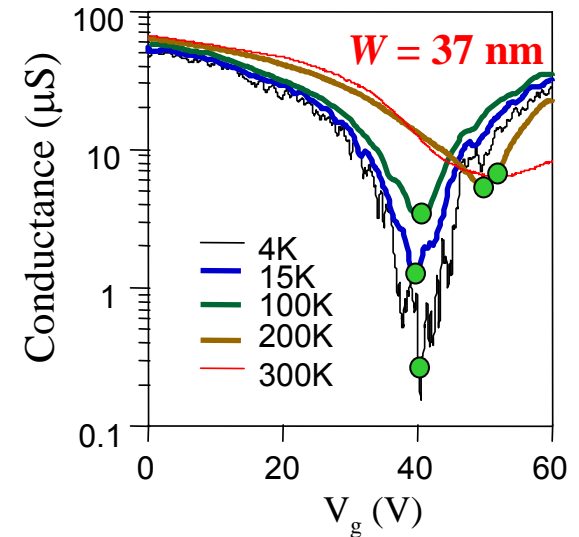


Variable Range Hopping in Graphene Nanoribbons



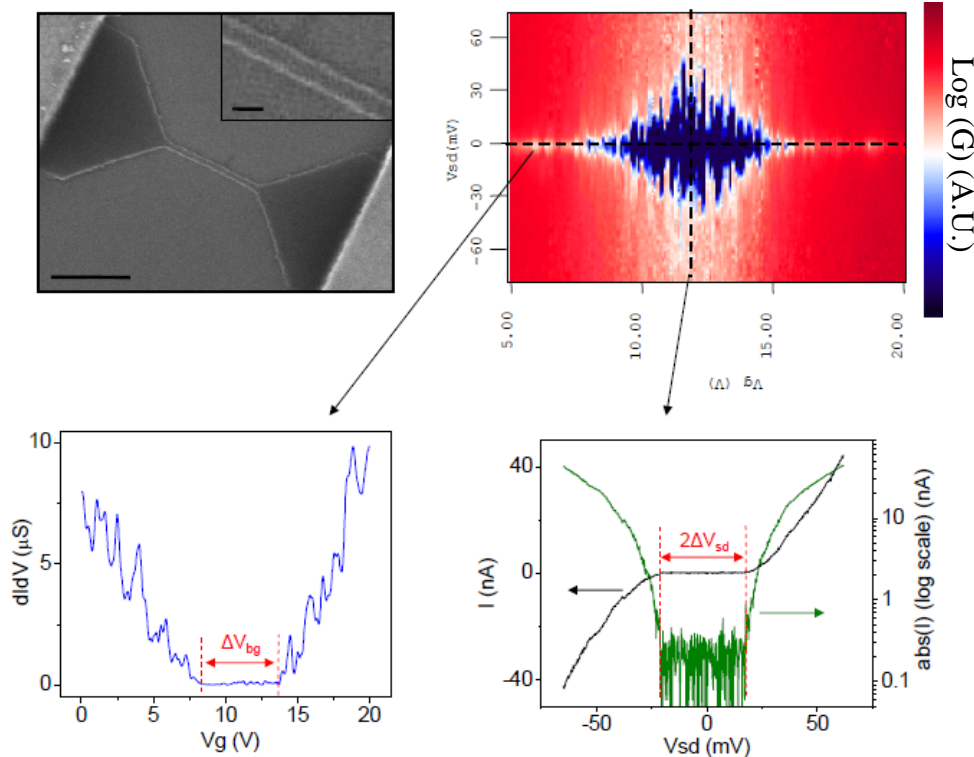
$$G_{\max} = G_0 \exp \left[- \left(\frac{T_0}{T} \right)^{\frac{1}{d+1}} \right]$$

d : dimensionality



Nature of Transport Gap in Graphene Nanoribbons

Transport Characterization: nanoribbons



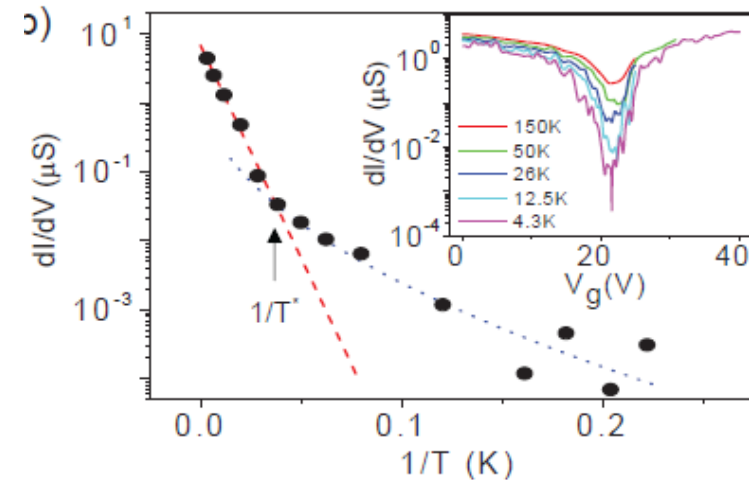
Graphene nanoribbons exhibits three different energy scales for energy gap formation due to the quantum confinement and edge disorders:

Δ_m : **mobility edges induced by edge disorder**

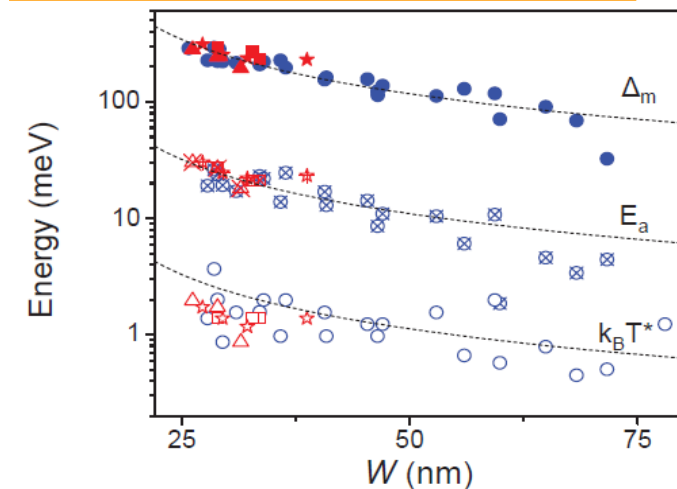
E_a : **Activation energy from the quantum confinement origin**

$k_B T^*$: **Hopping length to the localized states in gapped regime**

Temperature Dependent Transport

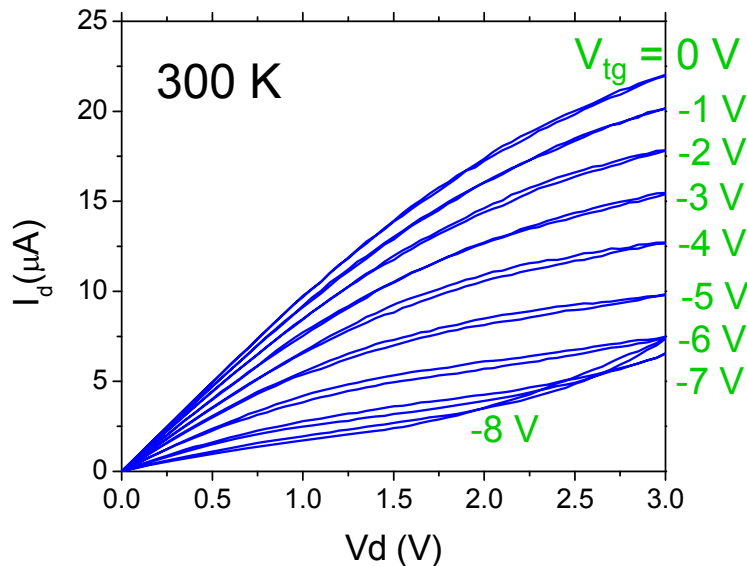
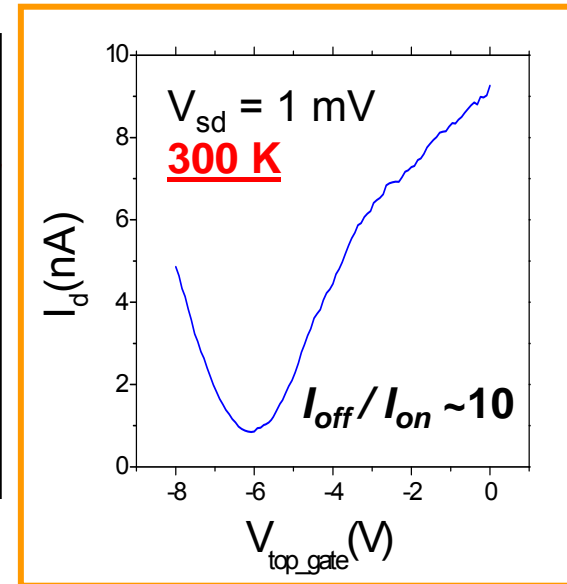
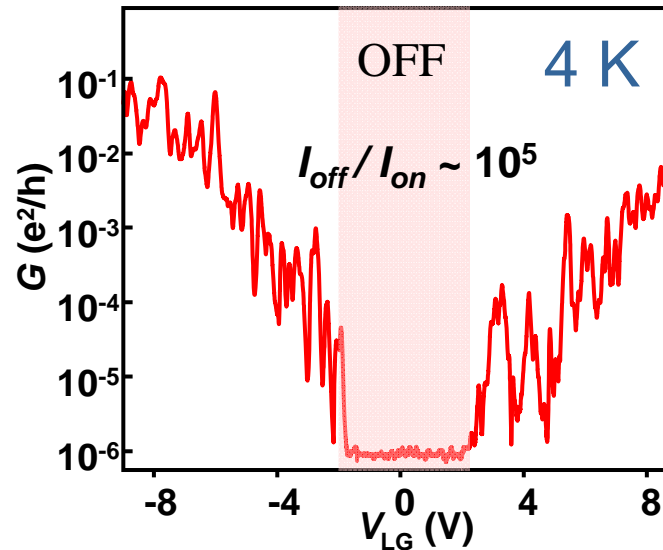
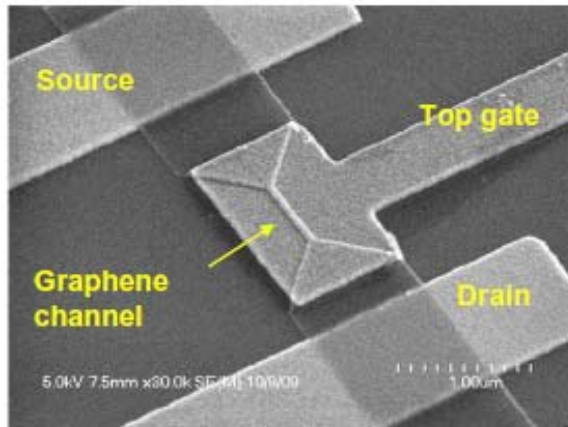


Energy Gap Scaling in Nanoribbons



Han *et al.*, Phys. Rev. Lett. (2010)

Top Gated Graphene Nanoribbon FET



Good

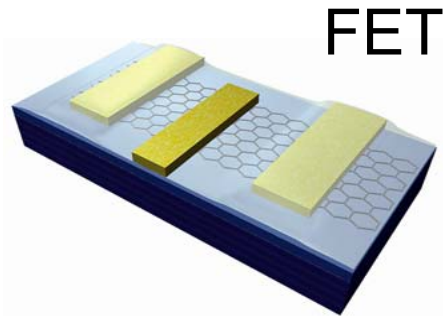
- High saturation velocity
 $V_{Fermi} = 1 \times 10^8 \text{ cm/s}$
 Silicon: $1 \times 10^7 \text{ cm/s}$
 GaAs: $0.7 \times 10^7 \text{ cm/s}$
- Operation current density $> 1 \text{ mA}/\mu\text{m}$

Bad

- Mobility: $\sim 500\text{-}1000 \text{ cm}^2/\text{Vsec}$
- On-off ratio: $\sim 10\text{-}30 \text{ @RT}$

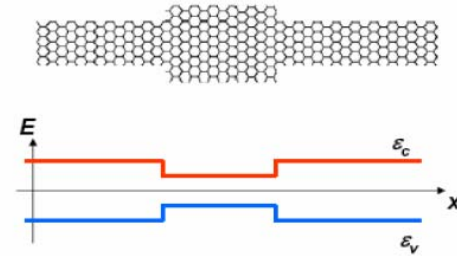
Graphene Electronics

Conventional Devices

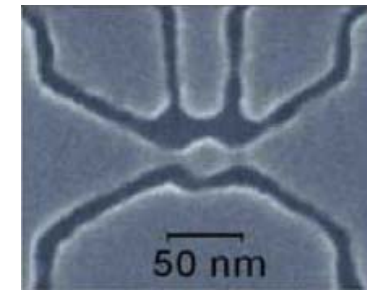


FET

Band gap engineered
Graphene nanoribbons

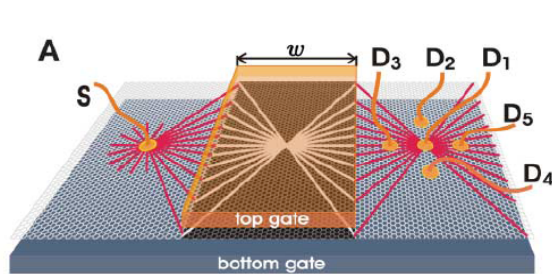


Graphene quantum dot



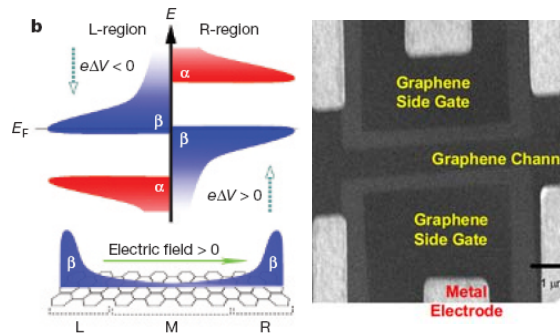
(Manchester group)

Nonconventional Devices



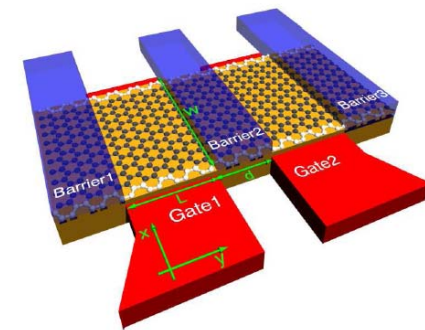
Graphene Veselago lens

Cheianov *et al. Science* (07)



Graphene Spintronics

Son *et al. Nature* (07)

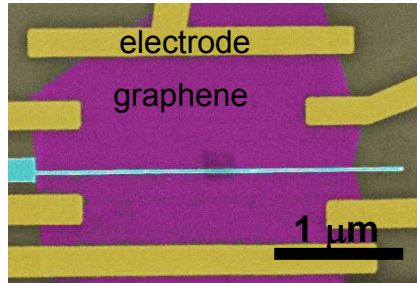


Graphene pseudospintronics

Trauzettel *et al. Nature Phys.* (07)

Transport Ballistic Graphene Heterojunction

Young and Kim (2008)



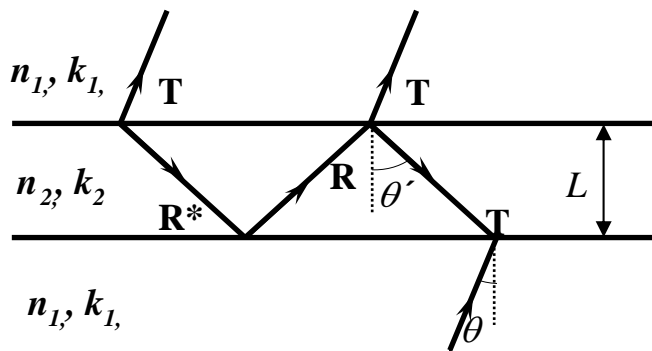
PN junction resistance

$$R = (\pi/2)(h/e^2)\sqrt{\hbar v / e|F_{pn}|}$$

Cheianov and Fal'ko (2006)

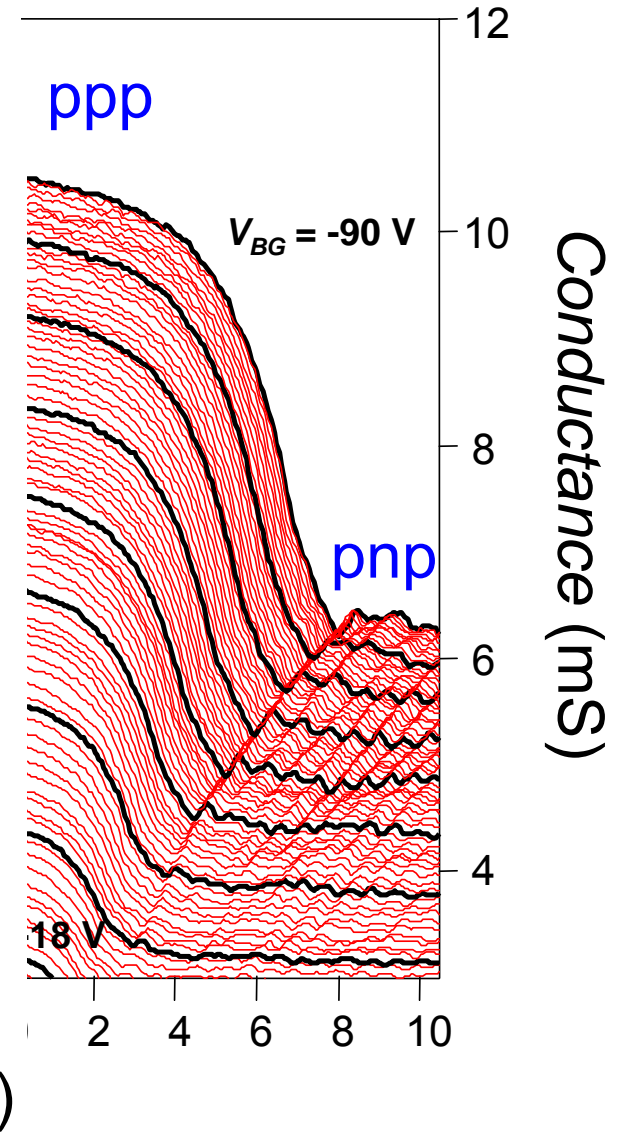
See also Shavchenko et al and Goldhaber-Gordon's recent PRL

Conductance Oscillation: Fabry-Perot



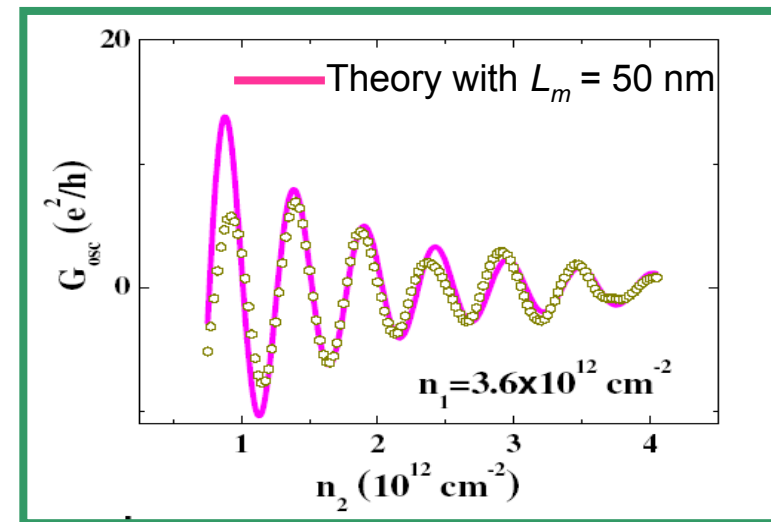
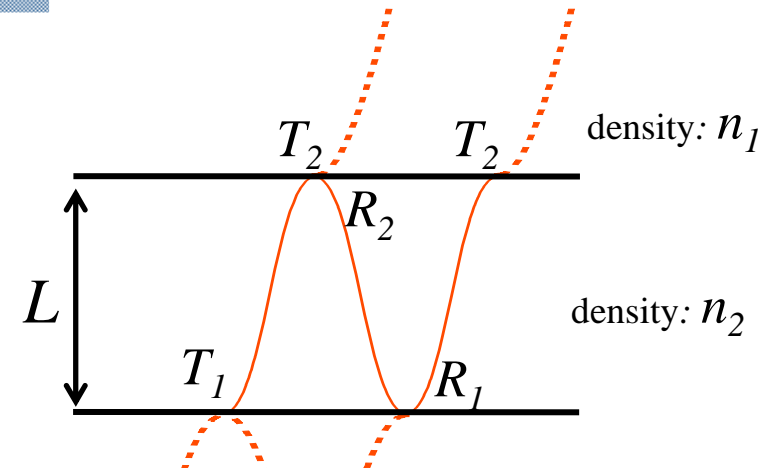
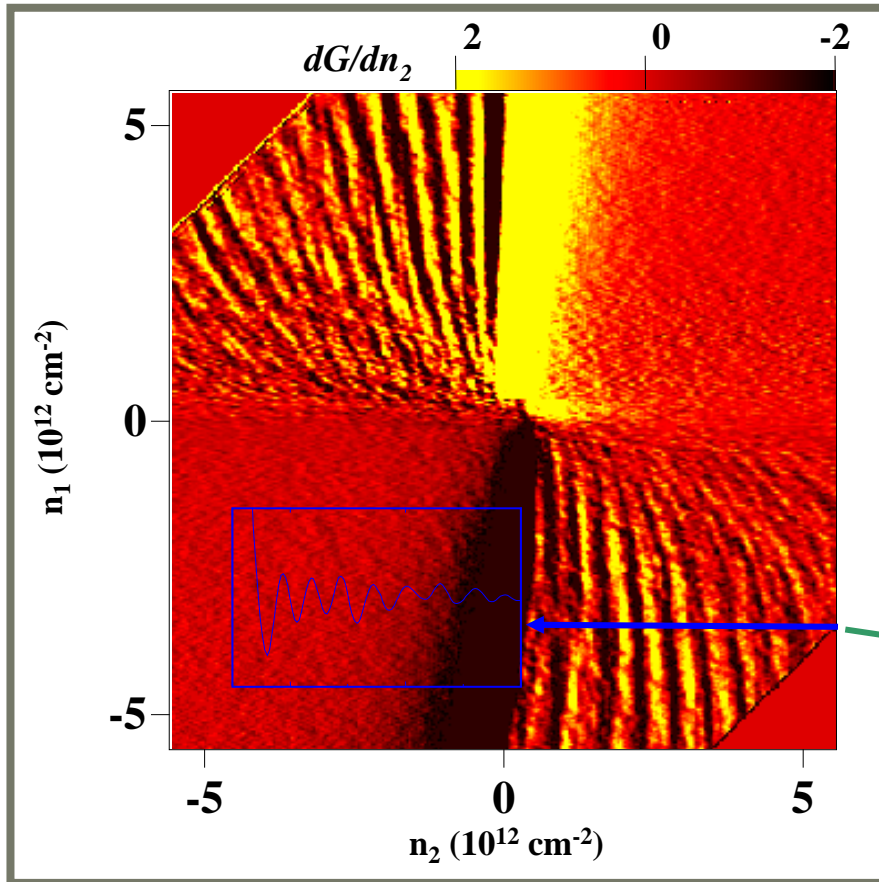
$$k_1/k_2 = \sin\theta' / \sin\theta$$

$$\Delta\phi = 2L / \cos\theta'$$



Fabry-Perot Oscillations in Ballistic Graphene Heterojunction

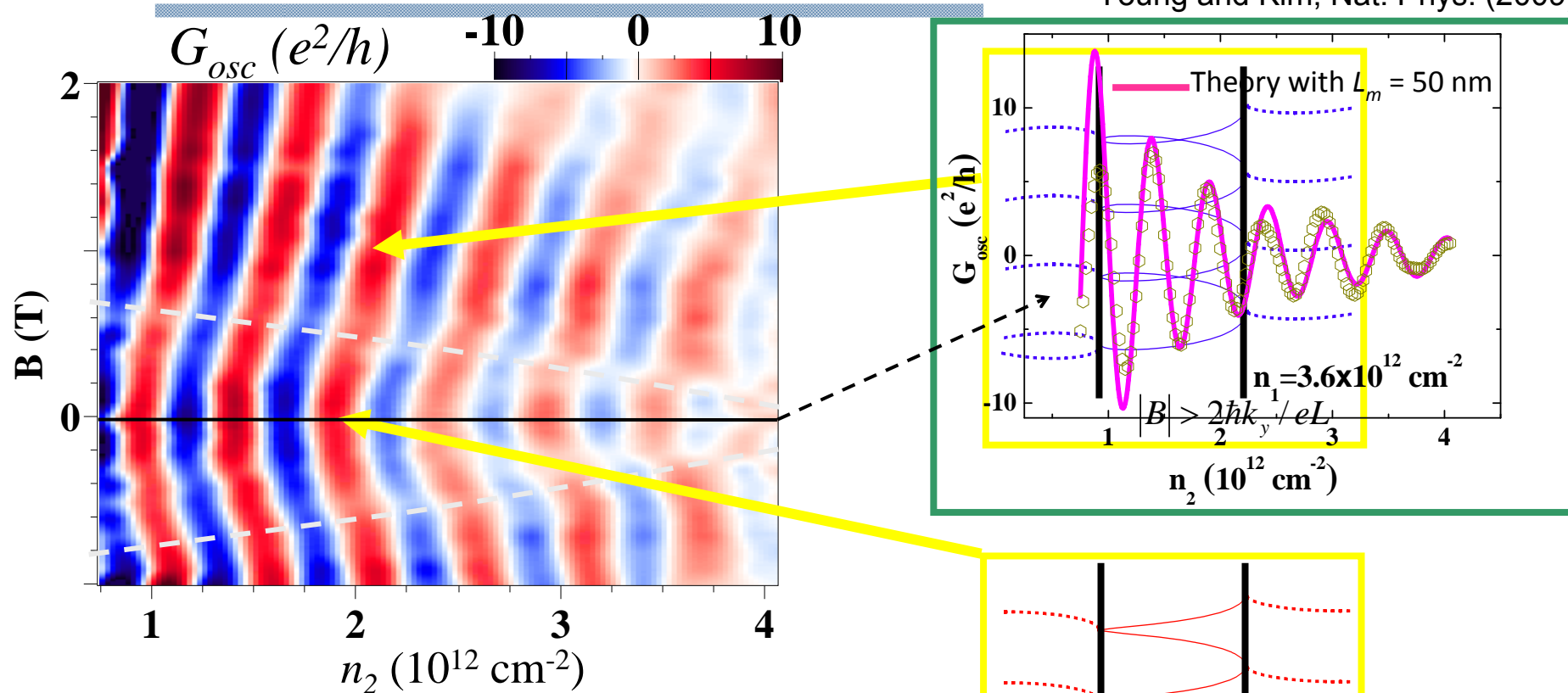
Derivative Map



$$G_{osc} \sim \frac{8e^2}{h} \sum_{k_y} |T_1|^2 |T_2|^2 |R_1| |R_2| \cos(\theta_{WKB}) e^{-4L/L_m}$$

Pseudo Spin Control with Magnetic Field

Young and Kim, Nat. Phys. (2009)



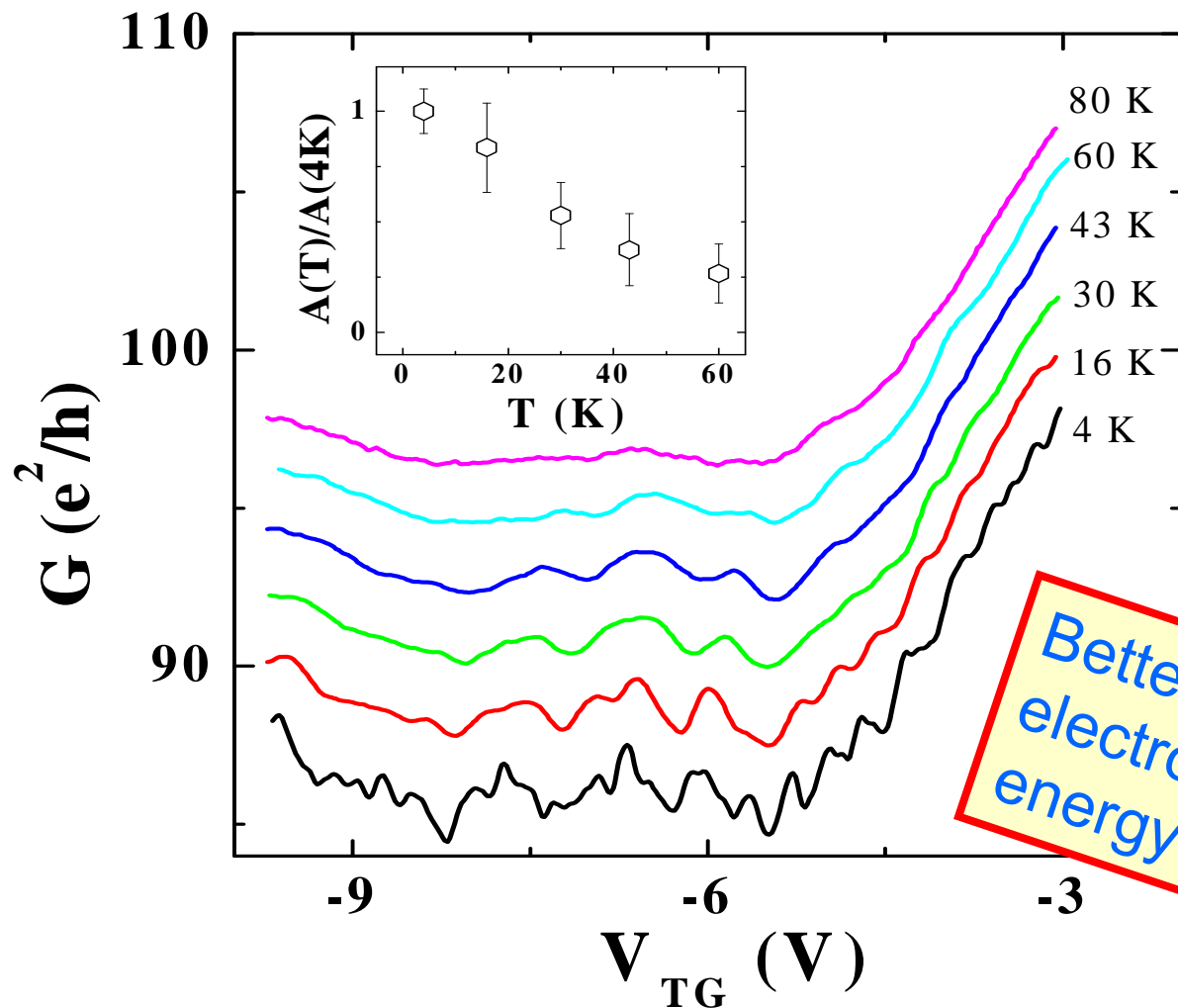
With increasing Magnetic field:

- * Oscillations phase shift
- * Abrupt phase at a certain magnetic field

Berry phase associated with pseudo spin

Levitov et al. (2008)

Temperature Dependence



- FP resonance to $\sim 80K$

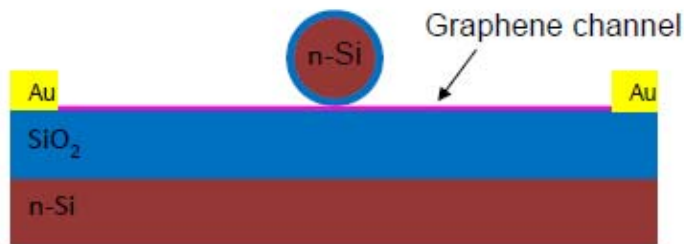
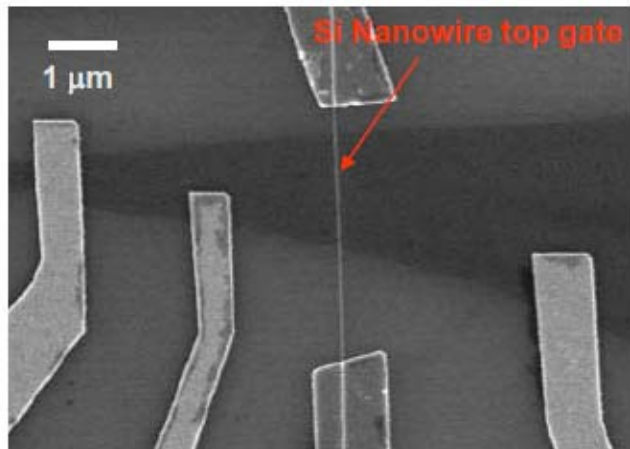
- Energy scale

$$T \approx \frac{\hbar v_F}{L} \approx 100K$$

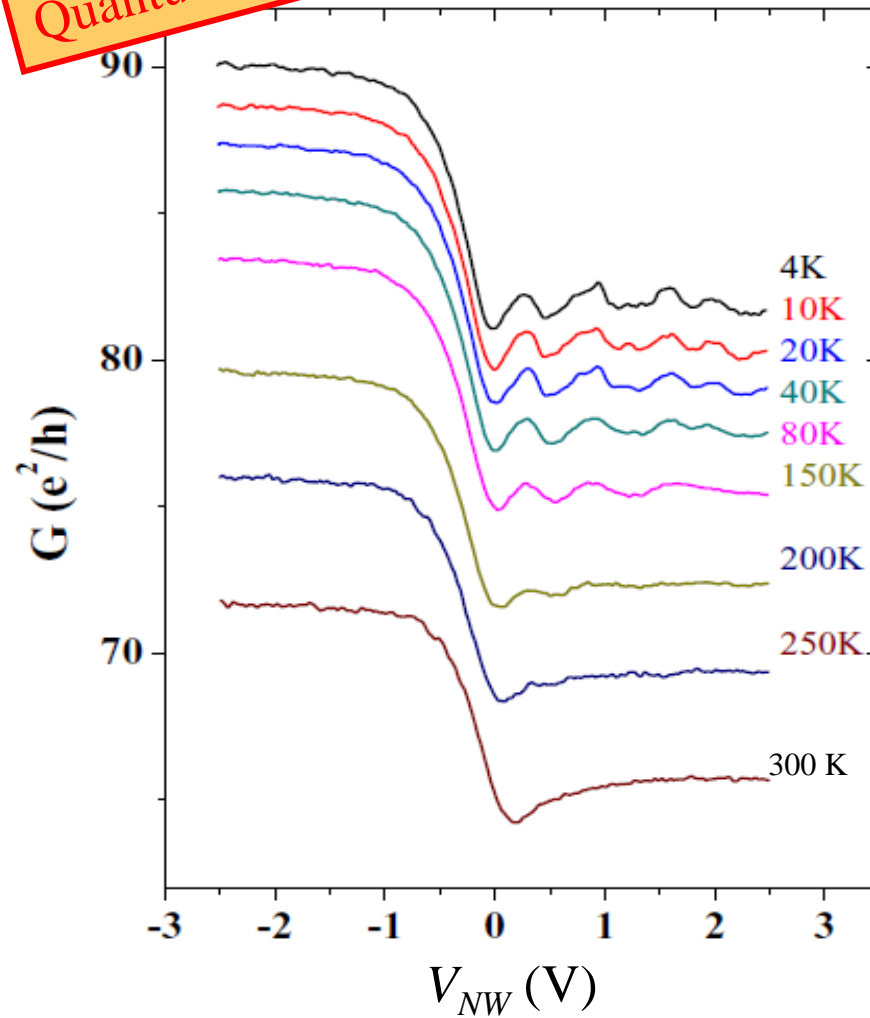
Better mobility and better electrostatic will make the energy scale larger!

Nanowire Top Gate: Ultimate Electrostatic

Quantum Oscillations at elevated temperatures

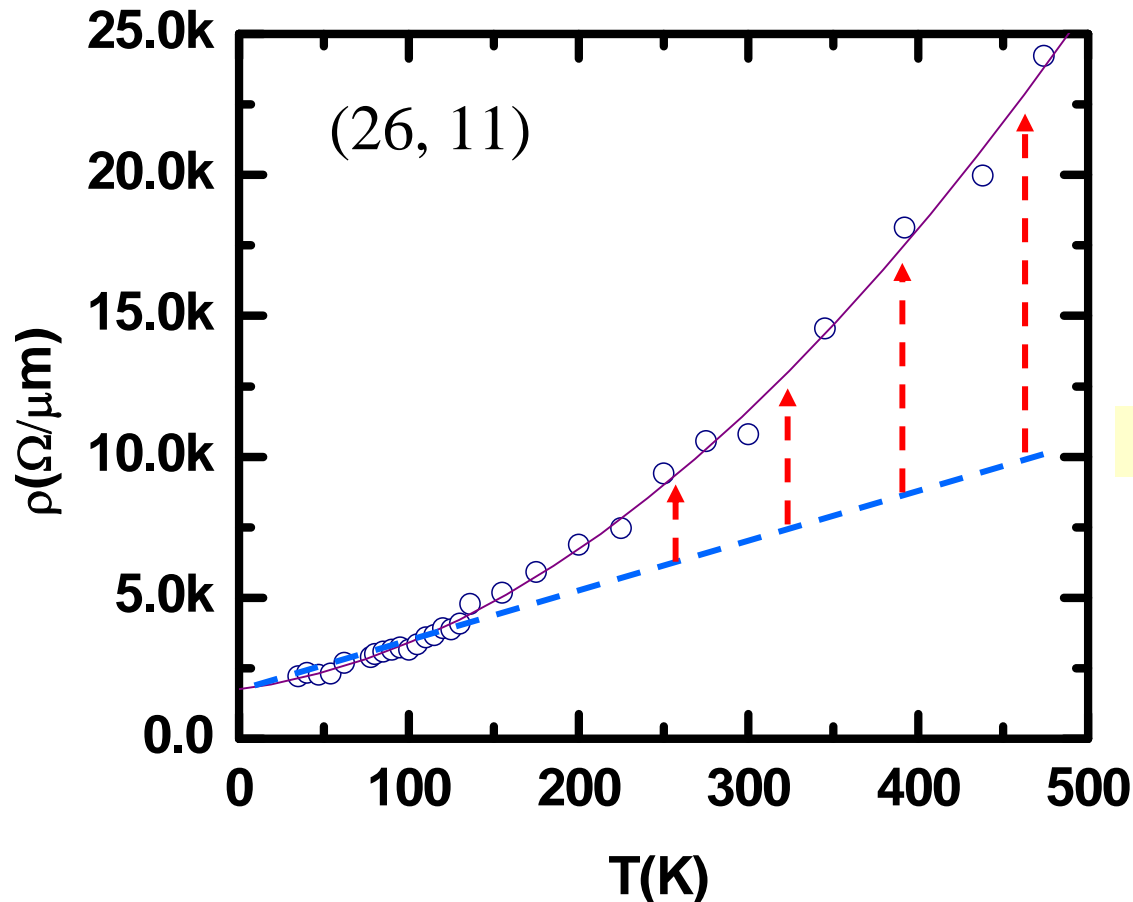


Si Nanowire: diameter ~ 25 nm
Natural SiO₂ dielectric ~ 2 nm



Temperature Dependence

Nanotube on SiO₂ substrate



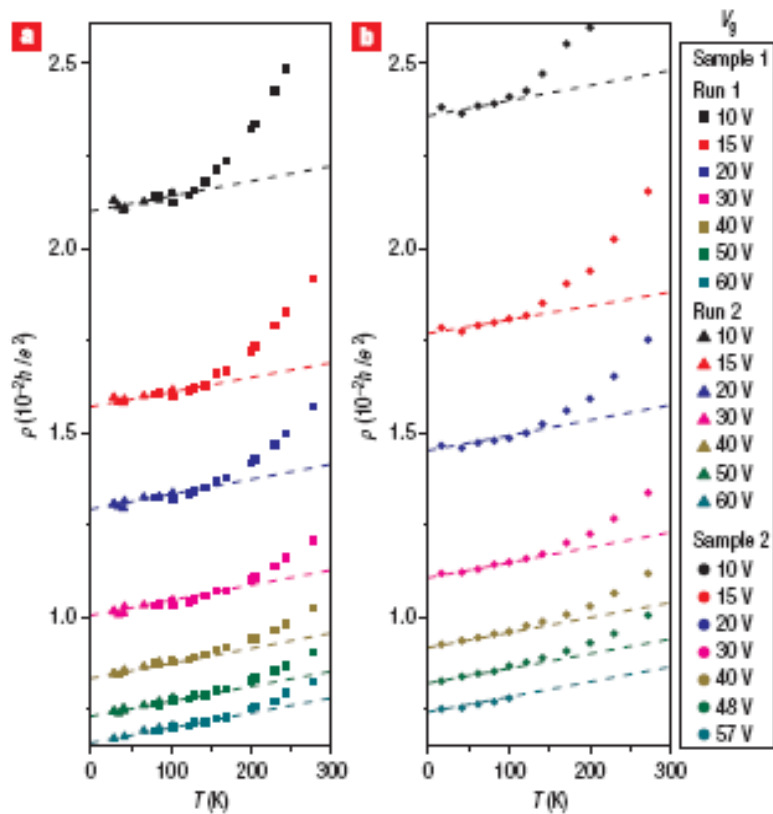
Super linear behaviors
for $T > 150$ K

Scattering due to acoustic phonons

$$\frac{1}{\tau_{ac}} = 2 \frac{2\pi}{\hbar} \Xi^2 \left(\frac{k_B T}{2\rho v_s^2} \right) \frac{1}{\hbar v_F}$$

Enhanced scattering activated $T > 150$ K

Optical phonons in substrates

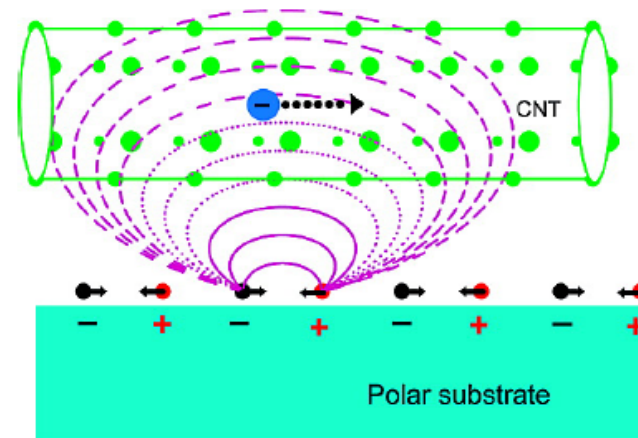


The Effects of Substrate Phonon Mode Scattering on Transport in Carbon Nanotubes

Vasili Perebeinos, Slava V. Rotkin, Alexey G. Petrov, and Phaedon Avouris

Nano Lett., 2009, 9 (1), 312-316 • DOI: 10.1021/nl8030086 • Publication Date (Web): 04 December 2008

Downloaded from <http://pubs.acs.org> on January 21, 2009



Transport in graphene
Chen et al. Nature Phys (2008)

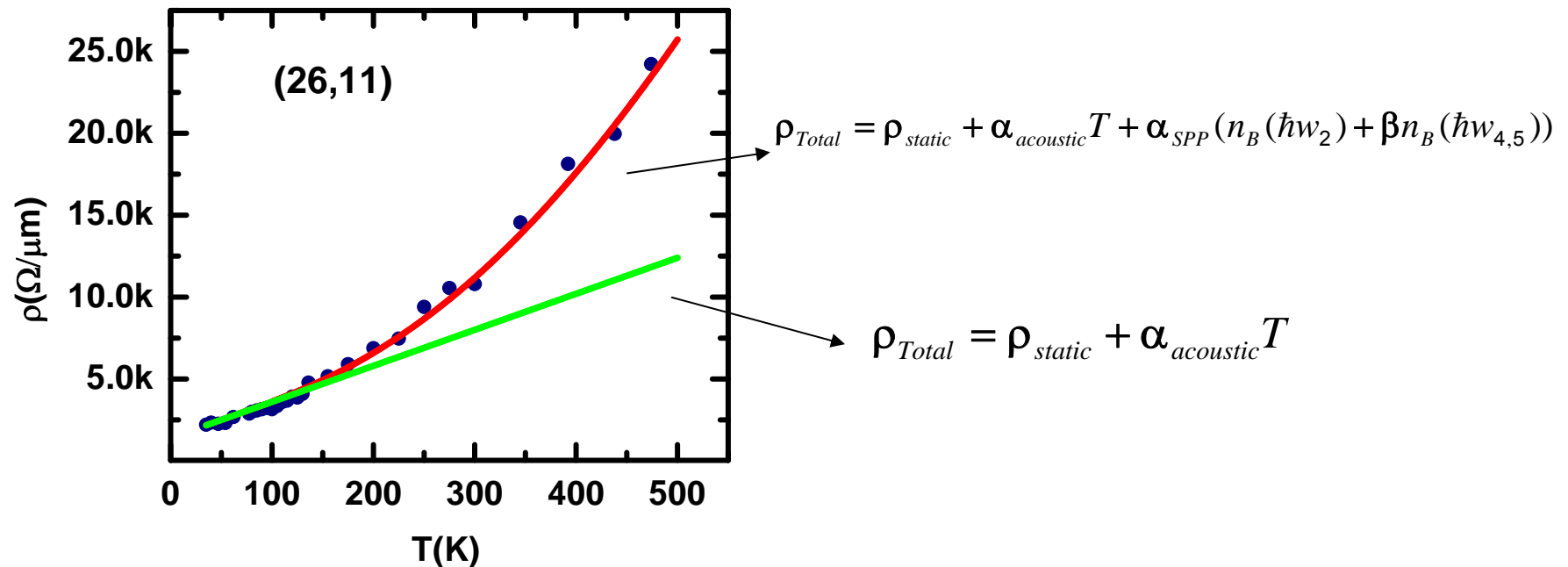
Optical phonons SiO₂ substrate is much softer ! (~ 30-50 meV)

Substrate Phonon Scattering Analysis

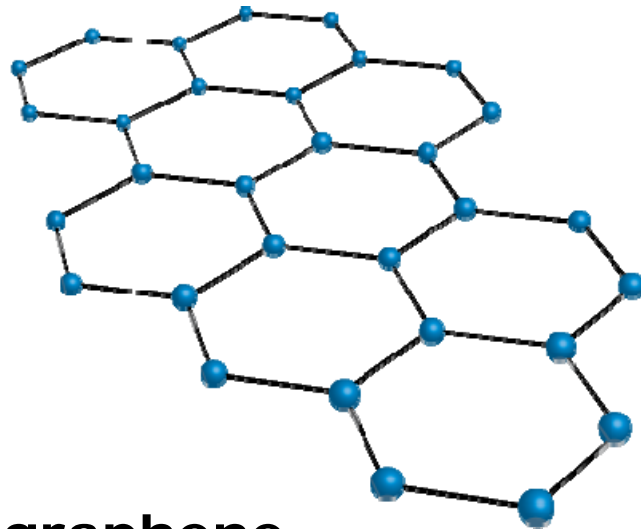
Perebeinos *et al.* Nano Lett. **9**, 312 (2009)

$$\rho_{Total} = \rho_{static} + \alpha_{acoustic} T + \alpha_{SPP} (n_B(\hbar\omega_2) + \beta n_B(\hbar\omega_{4,5}))$$

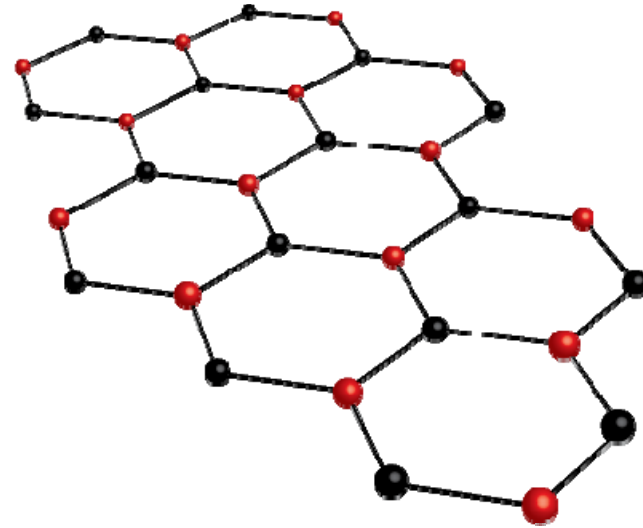
$$F_v^2 = \frac{\hbar\omega_{SO,v}}{2\pi} \left(\frac{1}{\epsilon_\infty + 1} - \frac{1}{\epsilon_0 + 1} \right) \quad \beta = \frac{(F_4^2 + F_5^2)}{F_2^2} \quad n_B(\hbar\omega_v) = \frac{1}{(e^{\hbar\omega_v/k_B T} - 1)}$$



hexa-Boron Nitride: Ideal Dielectric



graphene

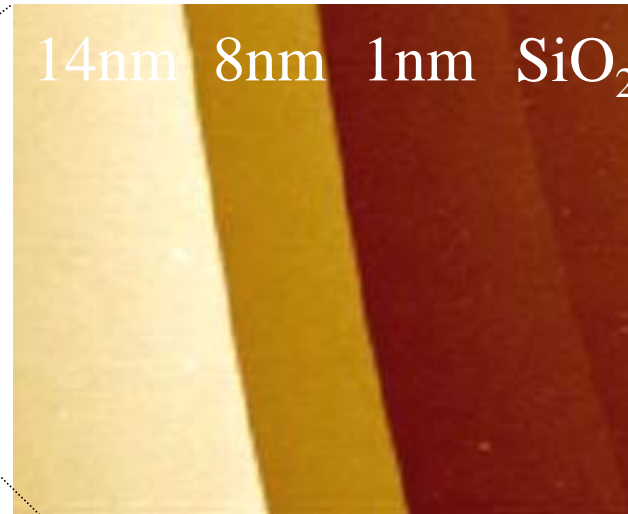
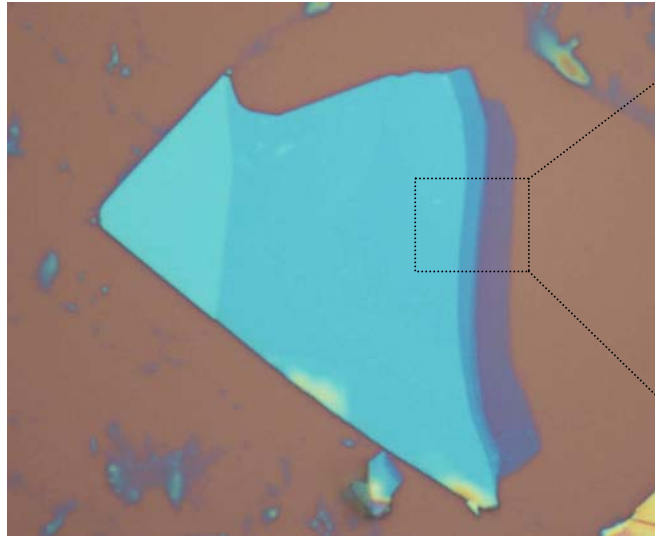


Boron Nitride

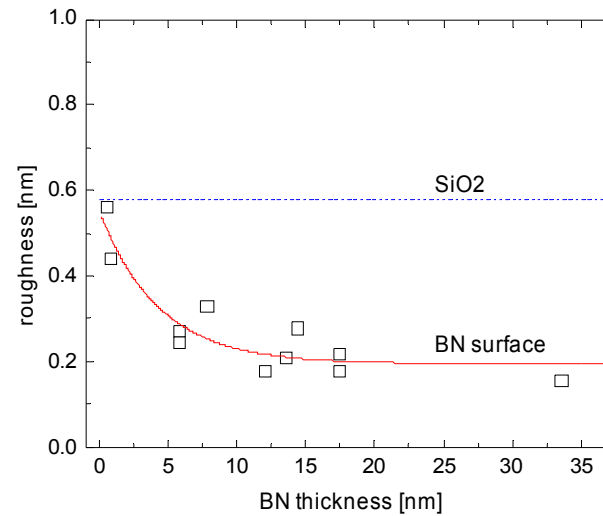
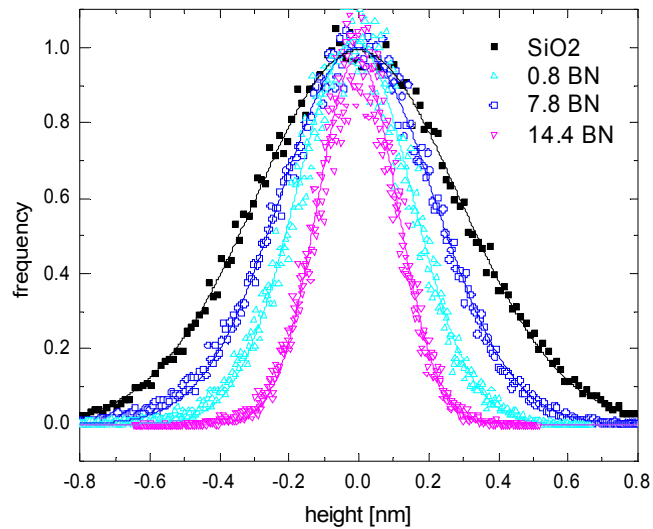
Comparison of h-BN and SiO₂

	Band Gap	Dielectric Constant	Optical Phonon Energy	Structure
BN	3.6 - 7.1 eV	~4	>150 meV	Layered crystal
SiO ₂	8.9 eV	3.9	59 meV	Amorphous

Mechanical Exfoliation of BN

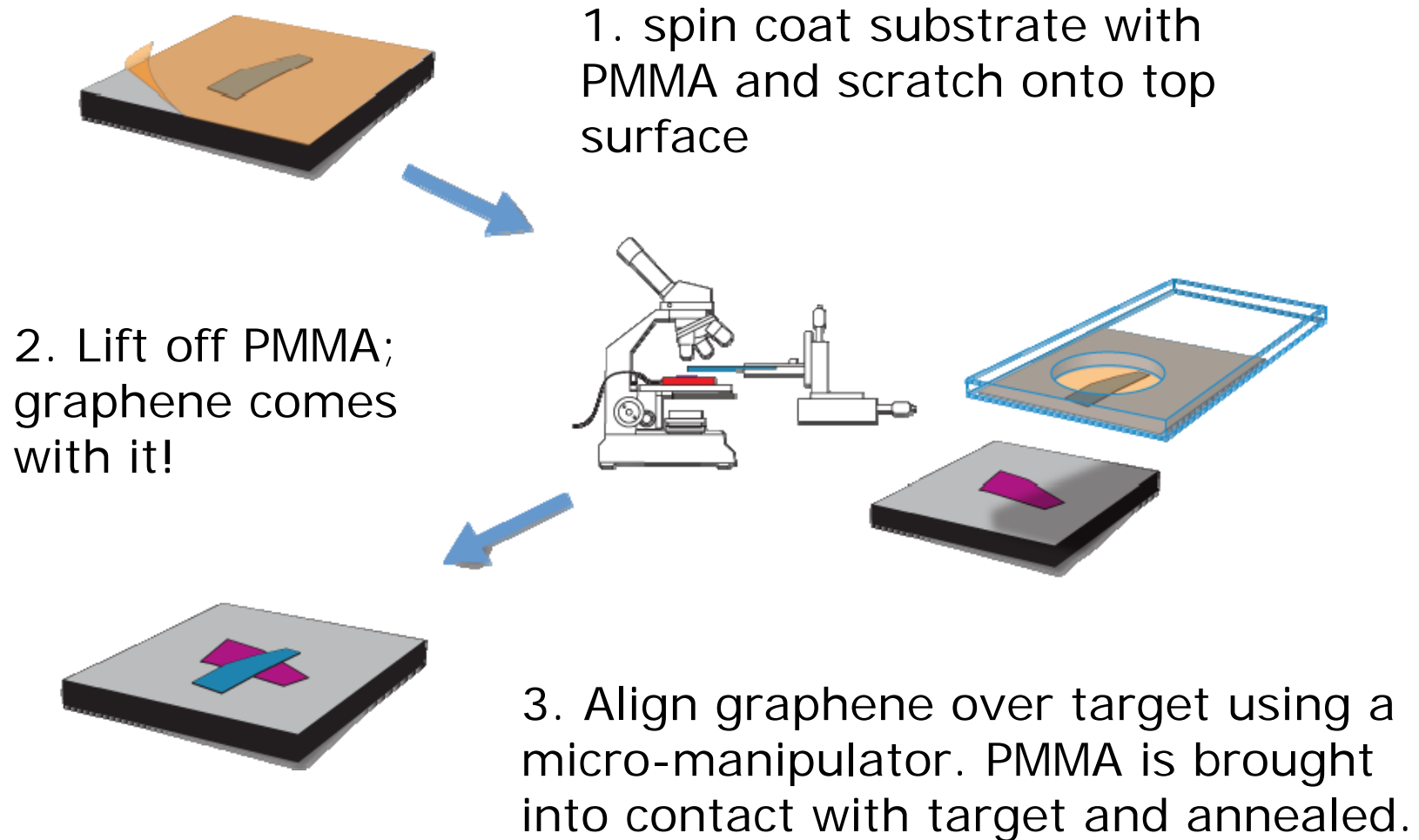


- Mechanically cleavable

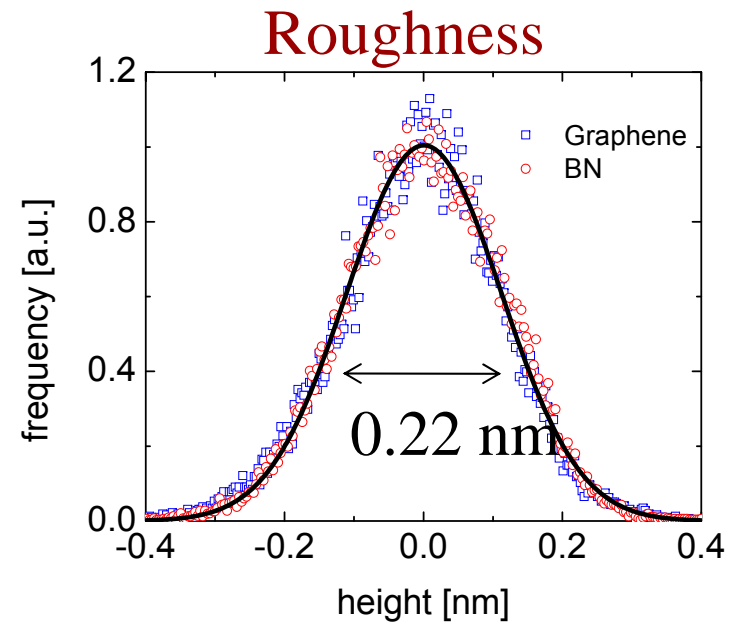
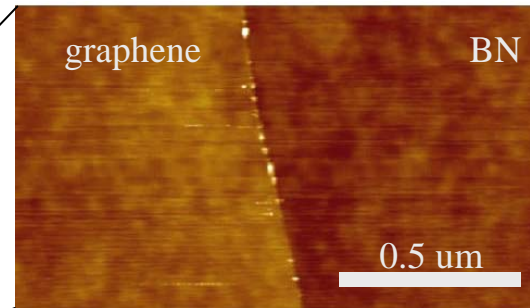
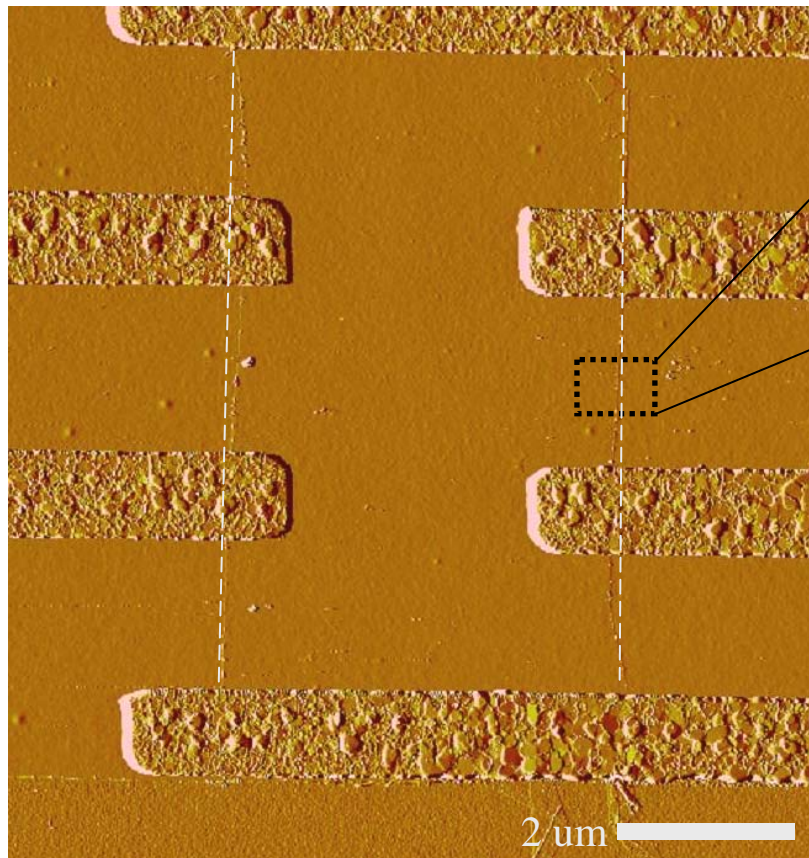


- Atomically flat

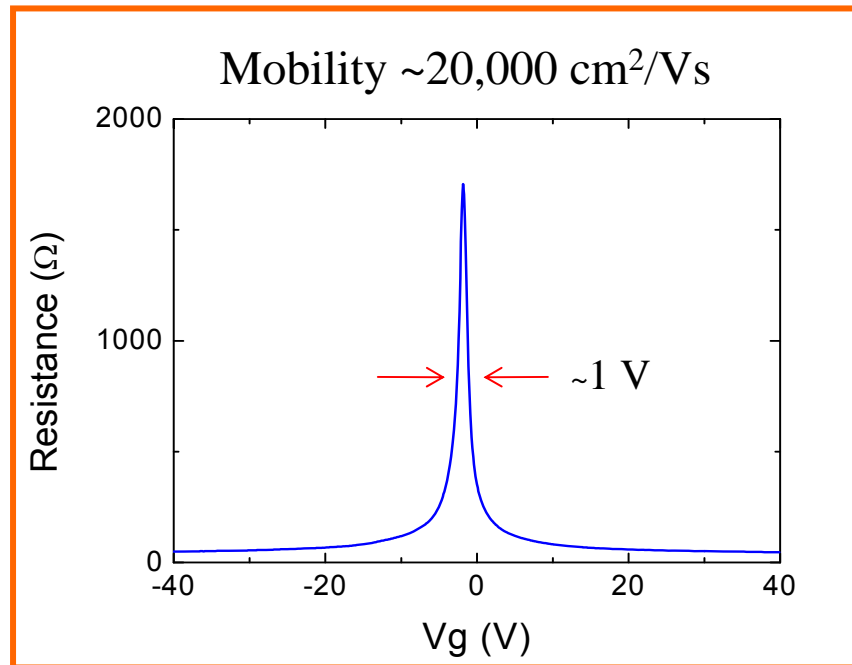
Precision Transfer Technique



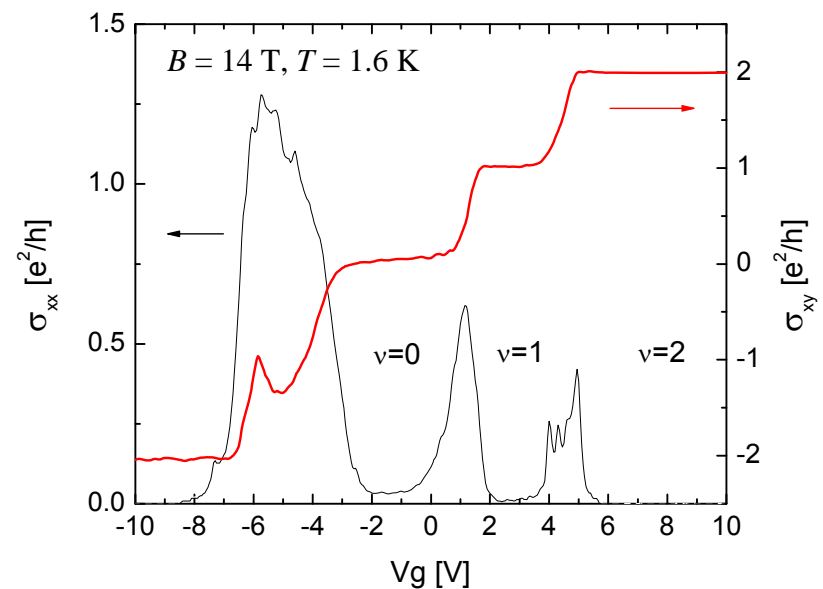
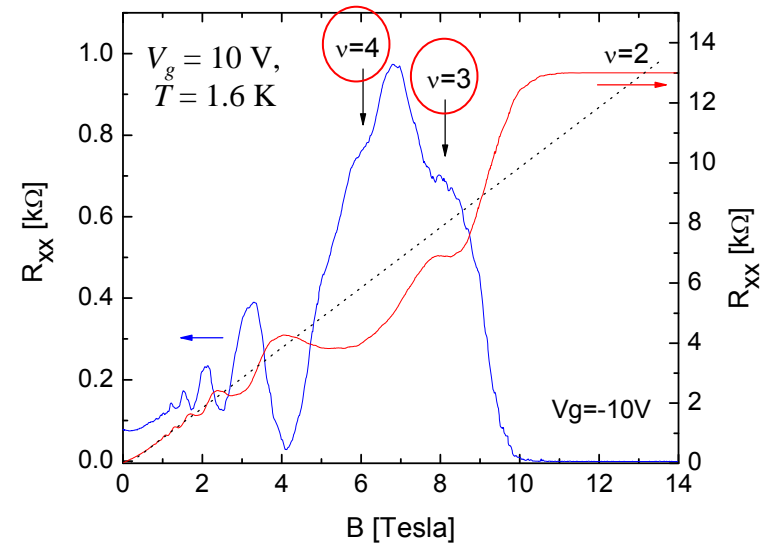
Graphene on h-BN is Flat!



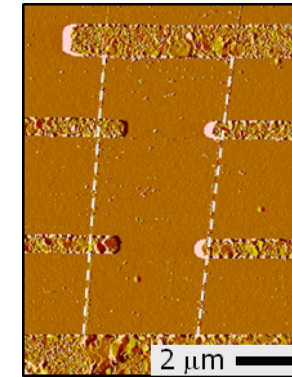
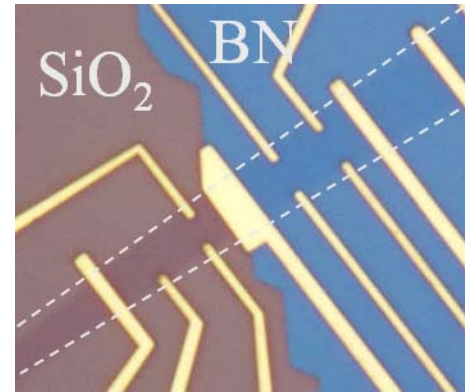
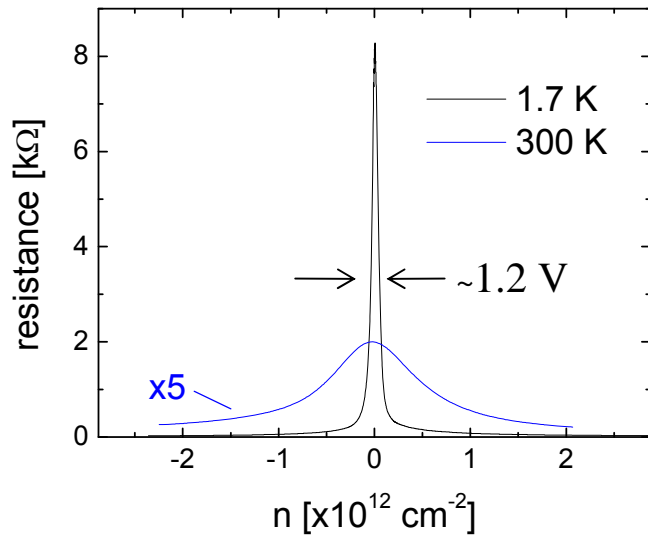
Transport in Graphene/h-BN



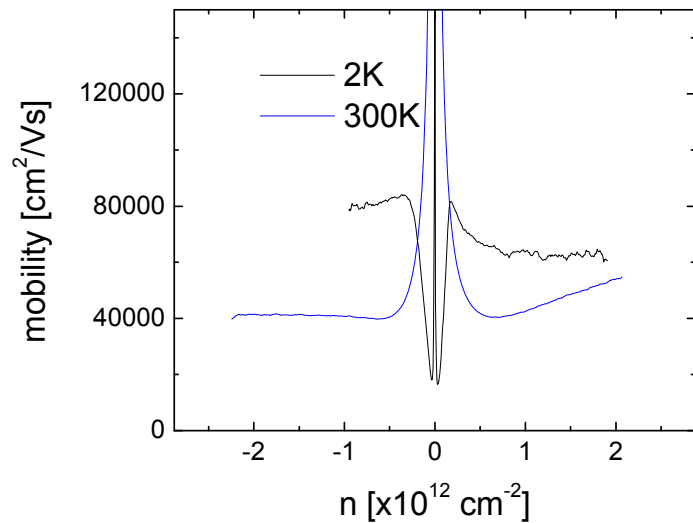
- Enhanced mobility on BN versus SiO_2 for the same flake
- Very narrow DP peak: reduced inhomogeneity.
- Reduced chemical reactivity (no appreciable doping by H/Ar annealing)



Bilayer graphene on Boron Nitride

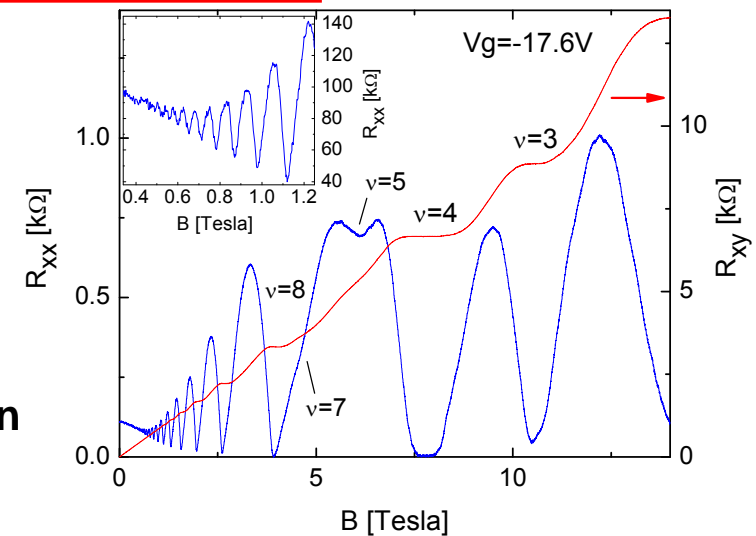


Bilayer graphene transferred over BN



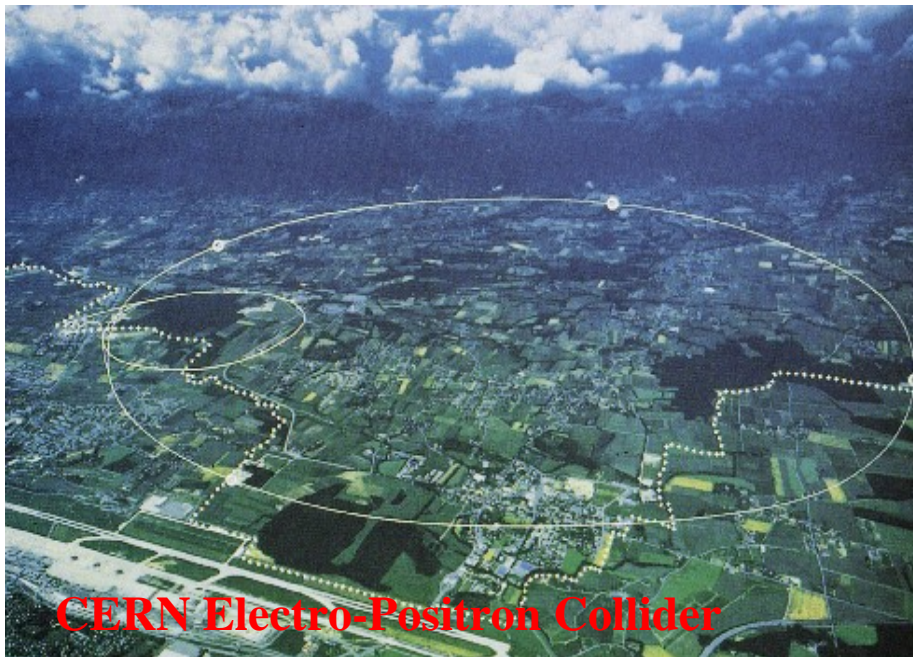
RT mobility > 40,000 cm^2/sec

SdH Oscillation

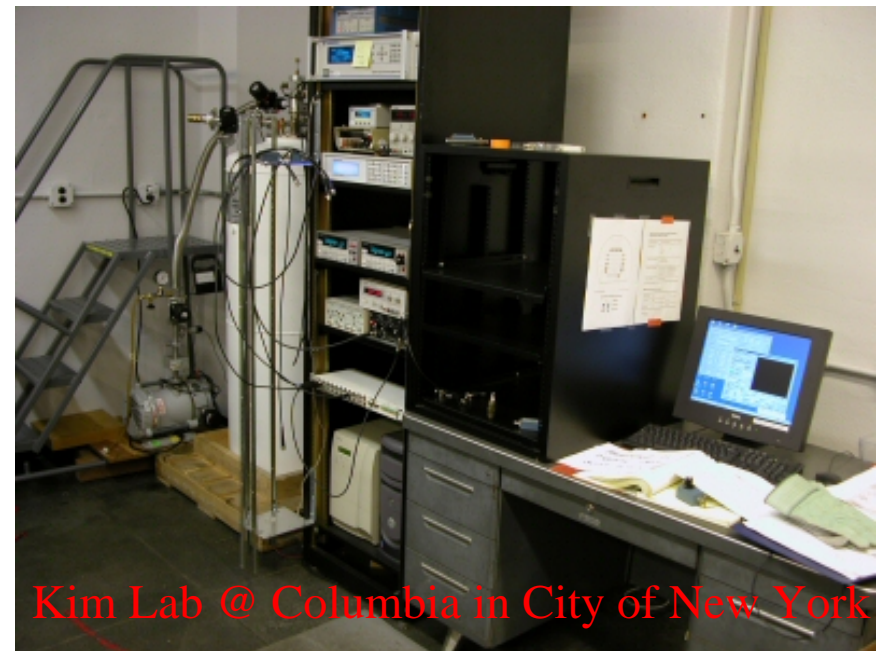


Conclusions

Relativistic QM: High Energy Physics



Quasi Relativistic QM: Low Energy Physics



Dirac Equation: $\tilde{H} = c^* \vec{\sigma} \cdot \vec{p}$

Acknowledgement

Special Thanks to:

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Dmitri Efetov
Fereshte Ghahari
Young Jun Yu
Namdong Kim
Kirill Bolotin
Vikram Deshpande
Paul Cadden-Zimansky

Collaboration:

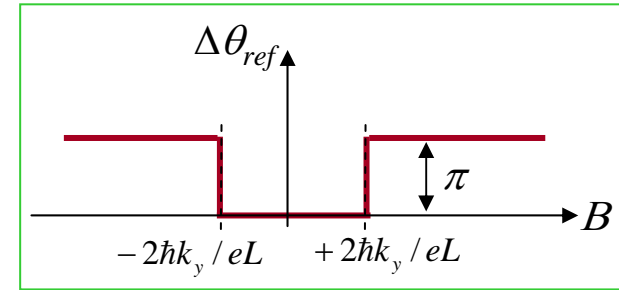
Stormer, Pinczuk, Heinz, Hone, Brus,
Nuckolls, Flynn, KS Kim, GC Yi, BH
Hong, A Chen



Funding:



FP resonances and Berry Phase



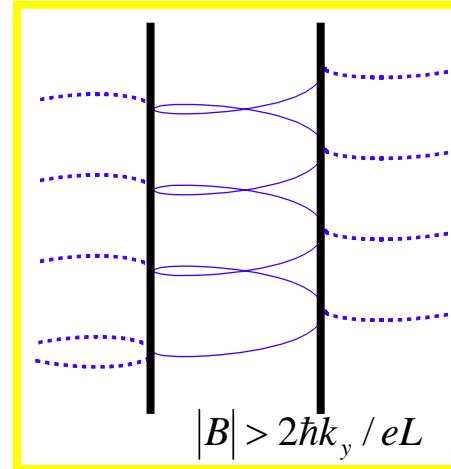
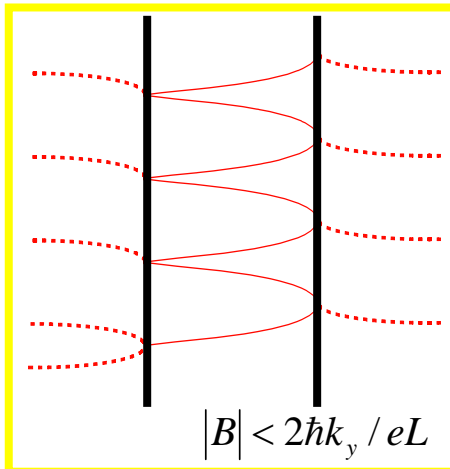
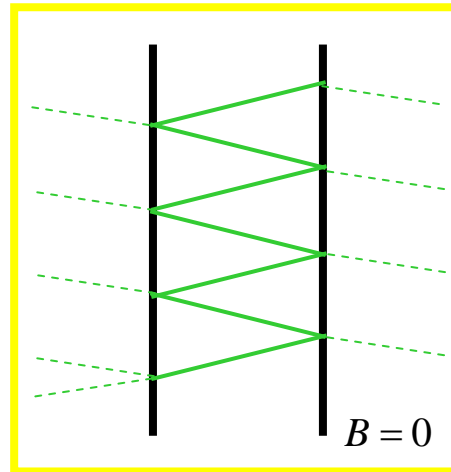
$$\theta_{WKB} = \Re \int_{-L/2}^{L/2} \sqrt{\pi |n(x)| - \left(k_y - \frac{e}{\hbar} Bx\right)^2}$$

$$\Delta\theta_{ref} = \pi \left[\theta\left(k_y + \frac{eBL}{2\hbar}\right) - \theta\left(k_y - \frac{eBL}{2\hbar}\right) \right]$$

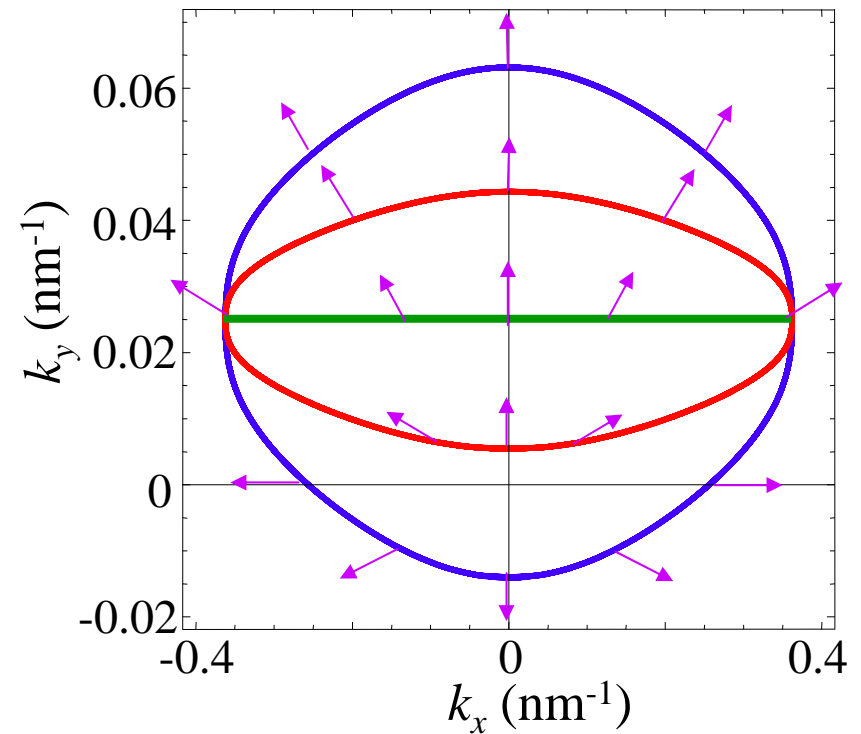
Real Space trajectories

Critical field

$$B_c = 2\hbar k_y / eL$$



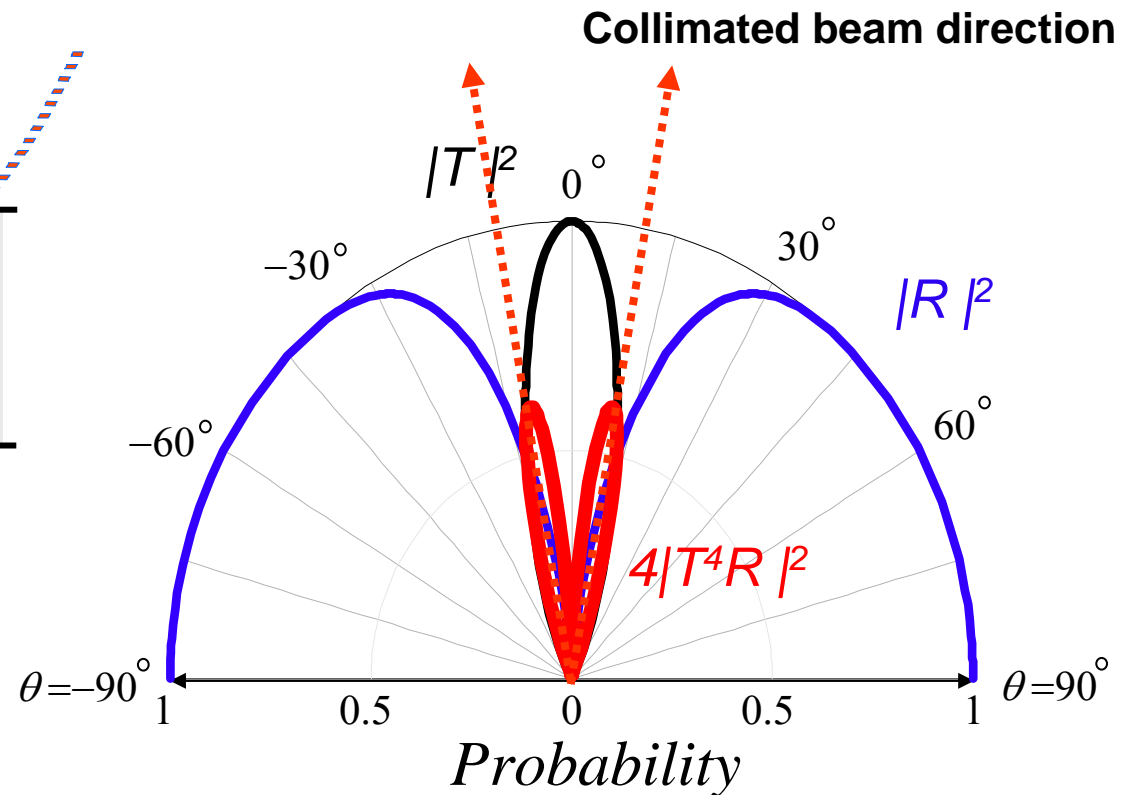
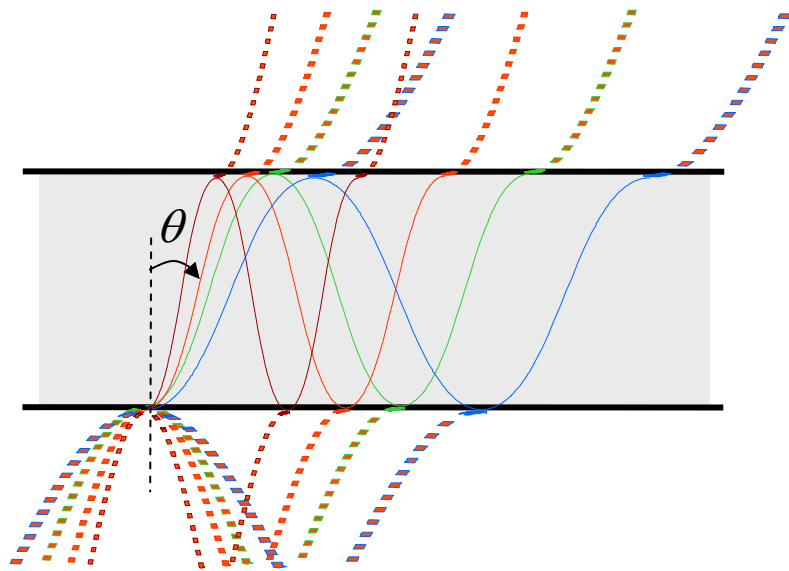
Momentum Space Trajectories



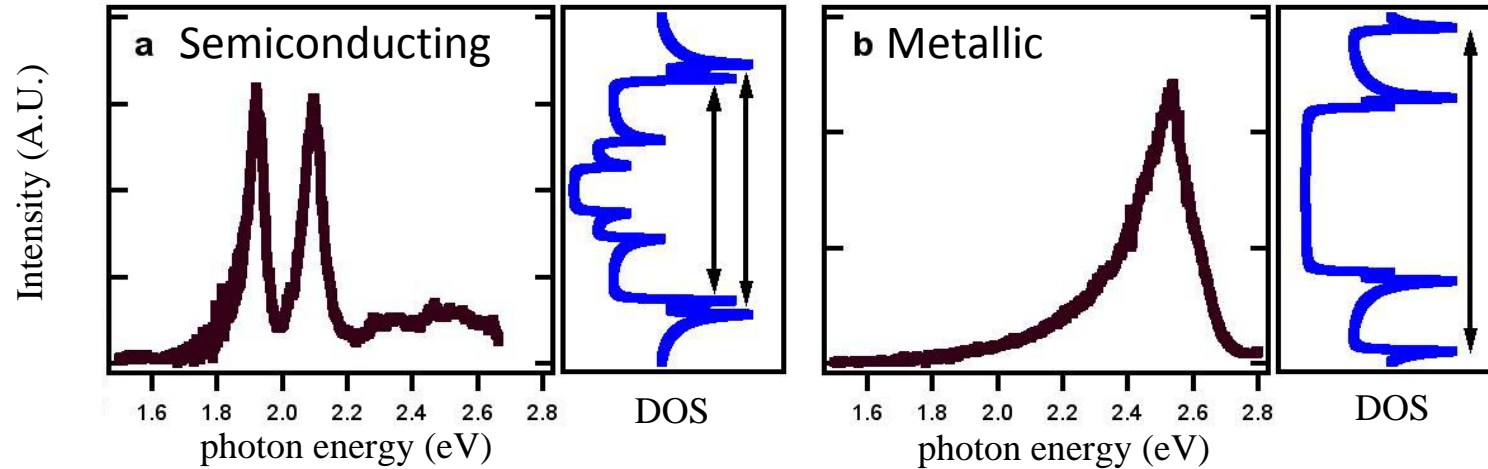
Wave Function Collimation in Diffusive Transport

$$G_{osc} \sim \frac{8e^2}{h} \sum_{k_y} |T_1|^2 |T_2|^2 |R_1| |R_2| \cos(\theta_{WKB})$$

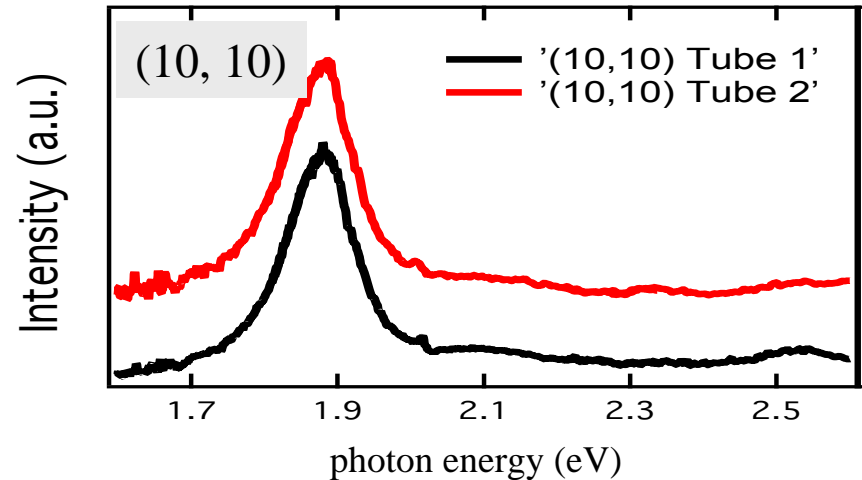
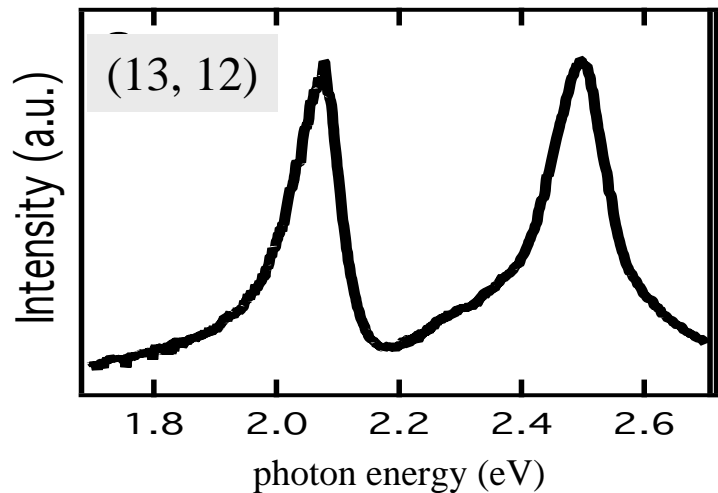
Diffusive transport outside of heterojunction regime



Rayleigh Light Scattering of Individual Tubes

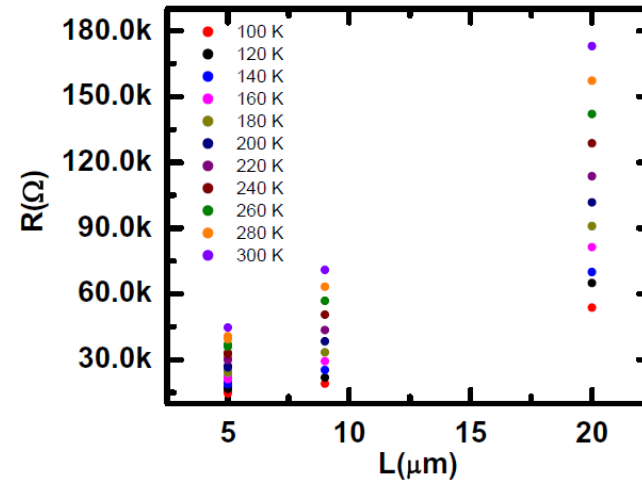
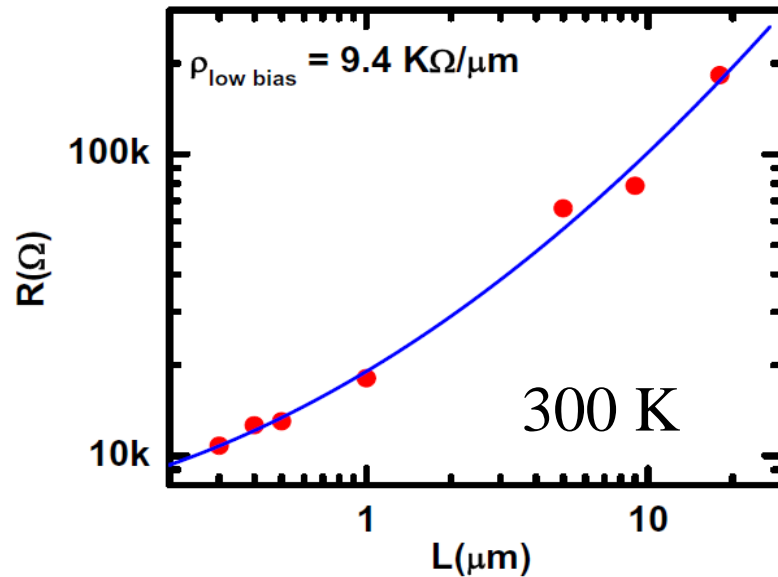


Structure can be analyzed from the Rayleigh Scattering Spectrum



Resistivity of (26, 11) Nanotubes

Temperature Dependence



1-dimensional resistance scaling

$$R(L) = \frac{h}{Ne^2} + \rho_{1d}L$$

Measurement of resistivity of known chirality in 4-500 K

