L5 Fabrication Techniques / Graphene Properties

Sunday, September 5, 2021 12:11 AM

Lecture notes by Ethan Minot, visiting from Oregon State University
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Nanoelectronics Class at Aalto University, Autumn, 2021.

Philosophy of the course - examine electron transport phenomena in small conducting structures.

The structures could be made out of

1. Normal metal wires
2. Superconducting wires
3. Semiconductors
4. Molecules
5. Graphene
6. Topological insulators

- Many practical considerations determine what is possible

- Ingenious fabrication tricks continue to open new possibilities

(sometimes invented by physicists and often coming from outside physics)

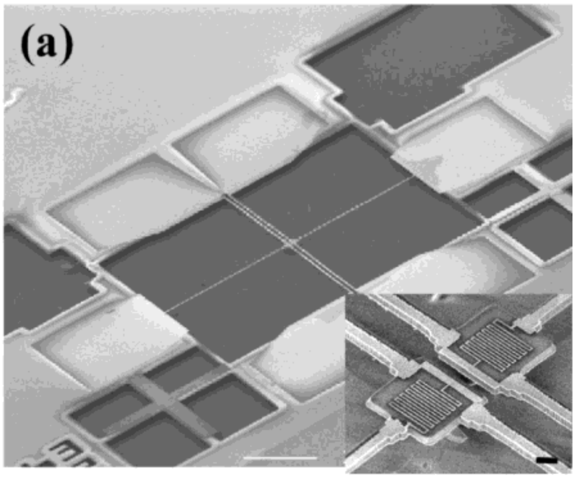
- Text book (section 1.1) has a nice overview of what was possible in 2012. Continues to evolve.

Part 1: Fabrication techniques

- Standard tools in semiconductor industry?
- Pristine surfaces and interfaces?
- Structure be protected from environment?

Some case studies…

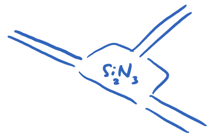
Kim et al. "Thermal transport measurements of individual multiwalled nanotubes" PRL 87, 215502 (2001)

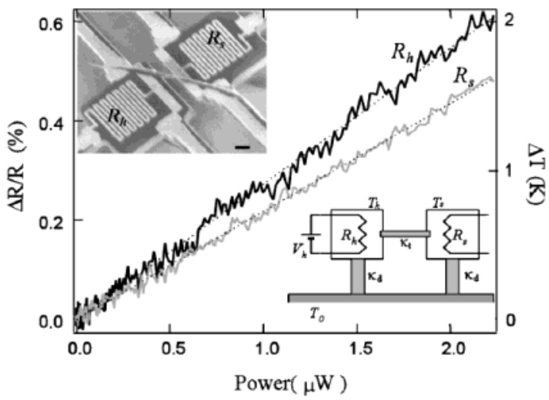


- Silicon wafer
- Photo lithography
- Anisotropic etching
- Isotropic etching. — eg. HF.

Need etch selectivity.

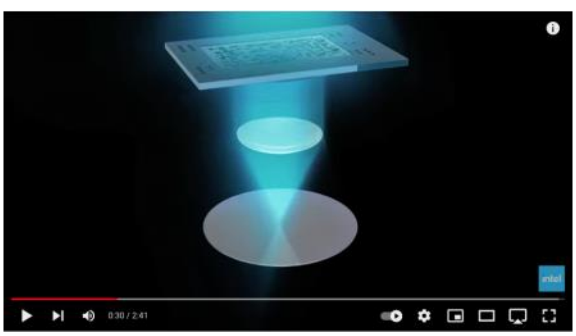
eg. SiO_2 vs Si_3N_4





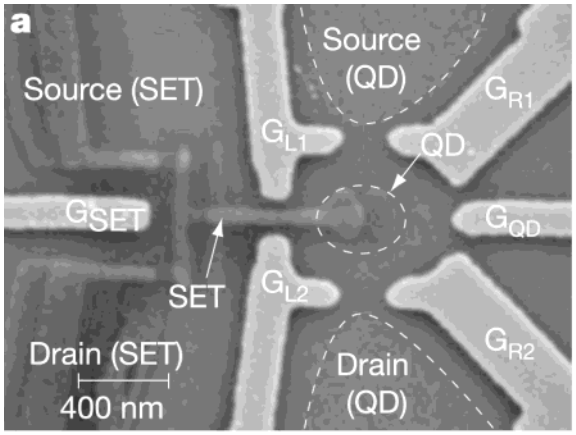
Piggy back on MEMS technology.

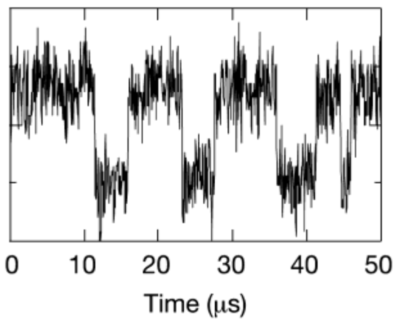
(industry techniques for making accelerometers)

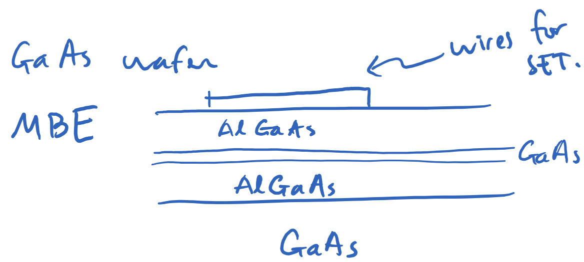


Video from intel: The making of a chip with 22nm/3D Transistors

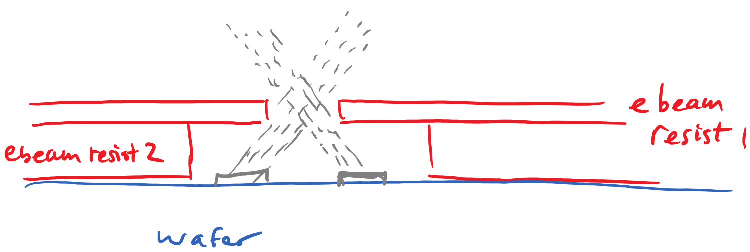
Lu et al. "Real-time detection of electron tunneling in a quantum dot" Nature 423 422 (2003)

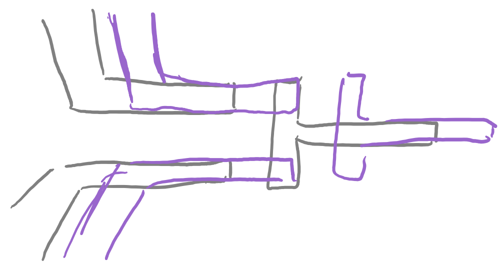




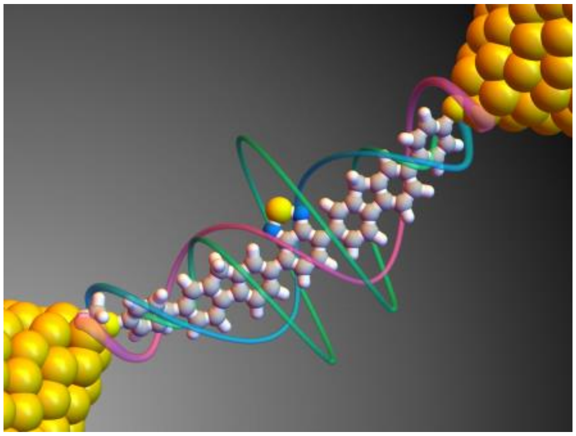


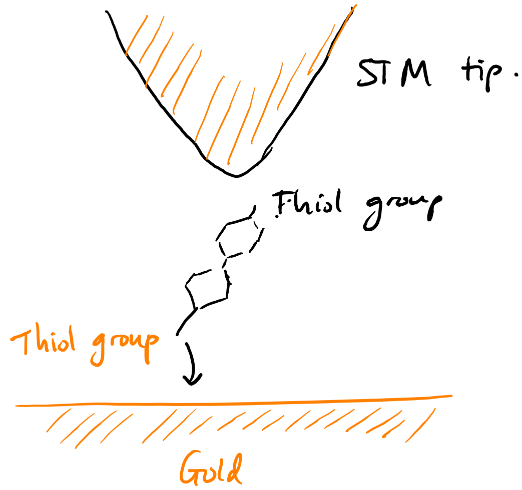
Angled evaporation and controlled oxidation

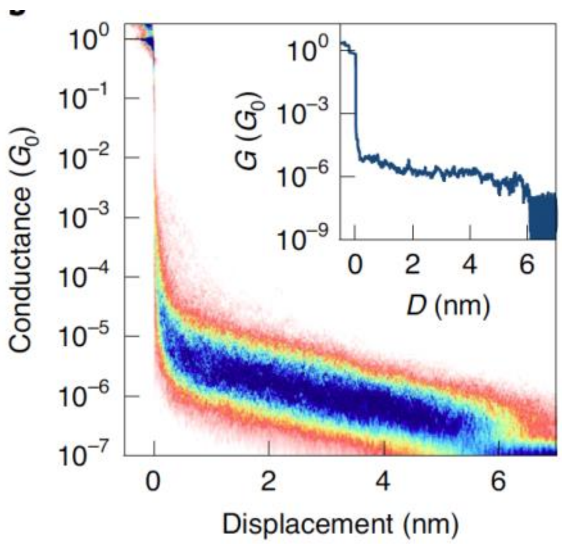


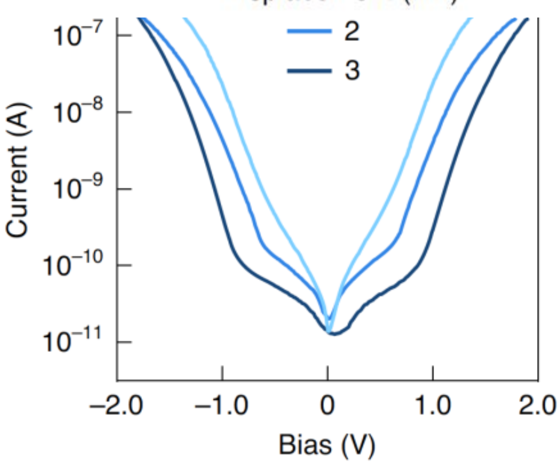


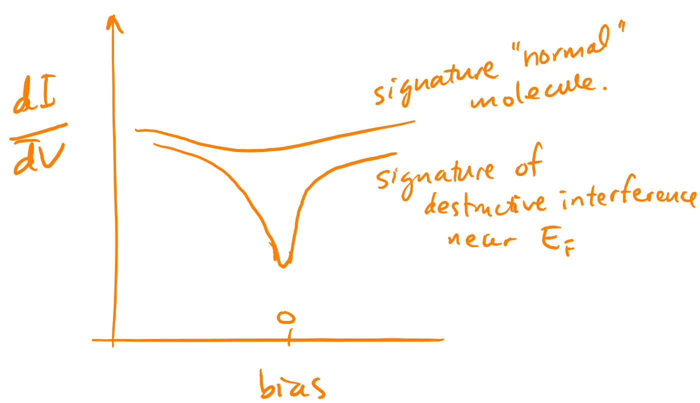
Greenwald et al. "Highly nonlinear transport across single-molecule junctions via destructive quantum interference" Nature Nanotechnology, 16 313 (2021)

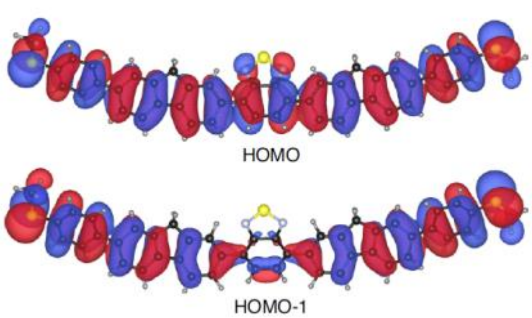



STM tip.
Thiol group
Thiol group
Gold

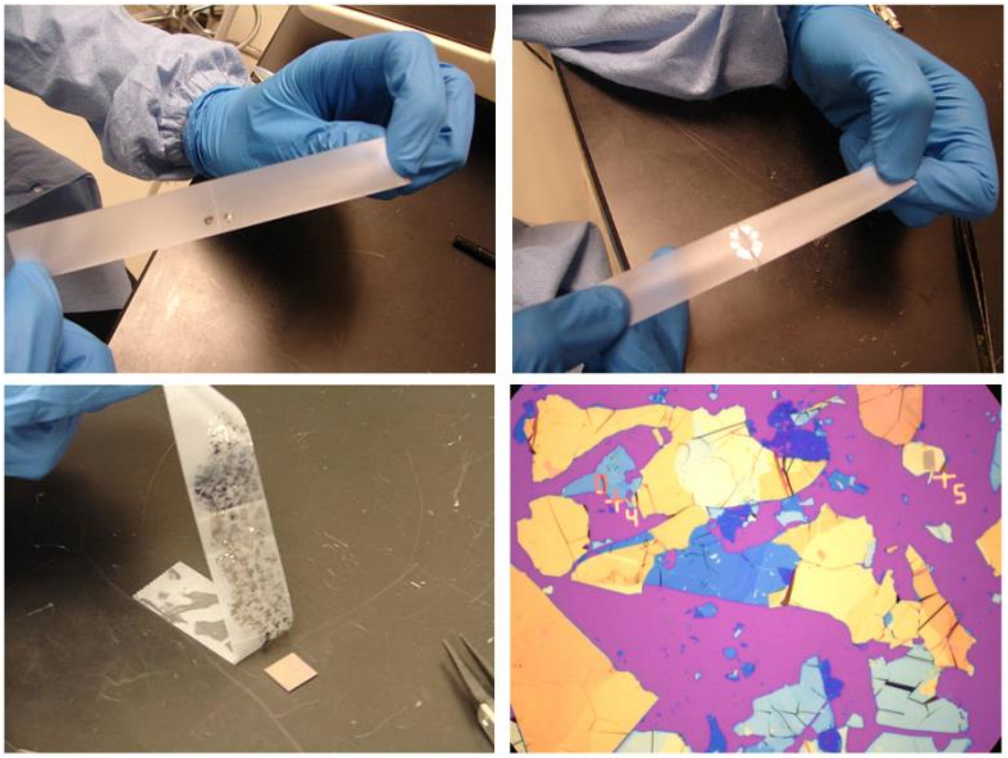

Conductance (G_0)
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
0
2
4
6
Displacement (nm)
G (G_0)
10^{0}
10^{-3}
10^{-6}
10^{-9}
0
2
4
6
D (nm)

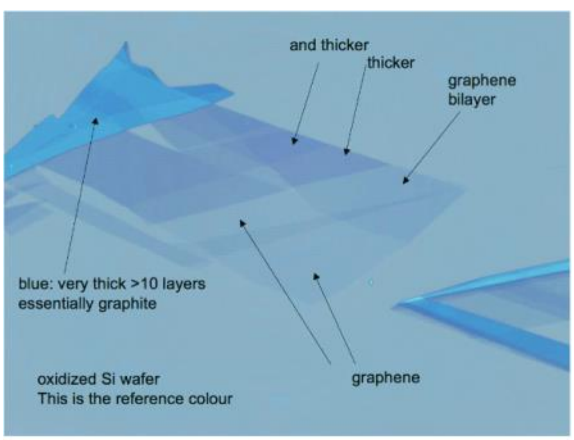

Current (A)
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
2
3
−2.0
−1.0
0
1.0
2.0
Bias (V)


$\frac{dI}{dV}$
signature "normal" molecule.
signature of destructive interference near E_F
0
bias

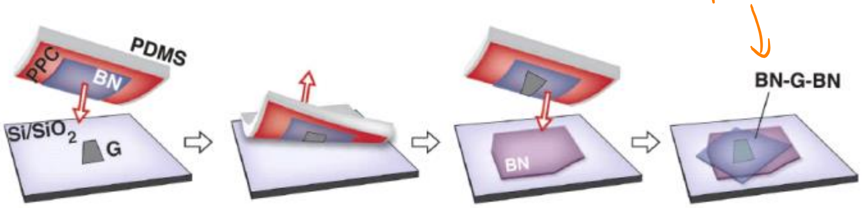

HOMO
HOMO-1

Wang et al. "One-dimensional electrical contact to a two-dimensional material" Science 342, 614 (2013)

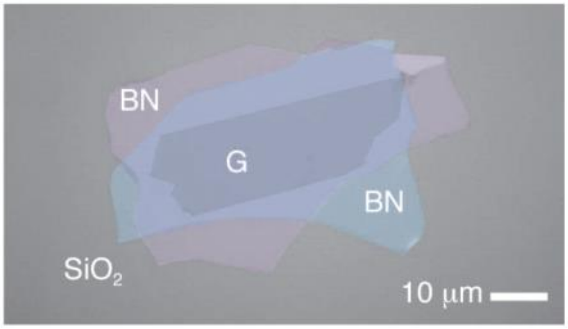




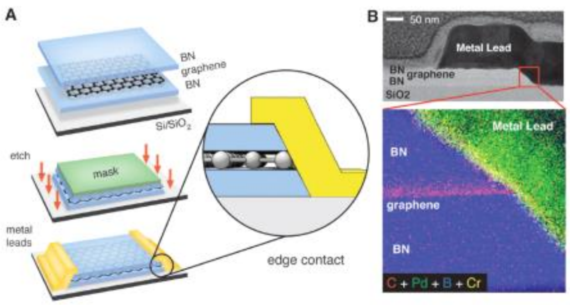
insulator.



Van der Waals

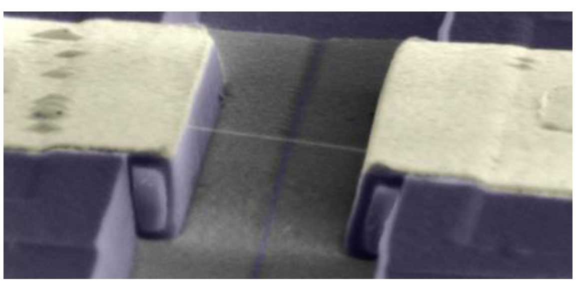


Stack of materials.

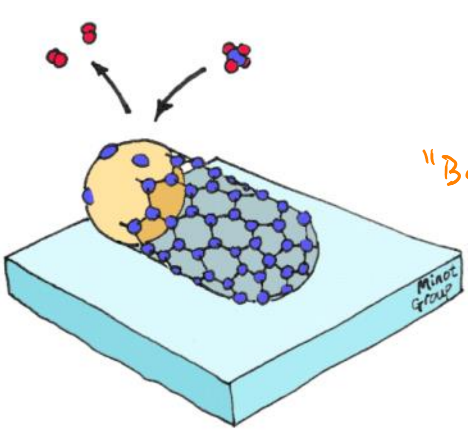


Room temp mobility 140,000 $\frac{cm^2}{V \cdot s}$

Lotfizadeh et al. "Bandgap-dependent electronic compressibility of carbon nanotubes in the Wigner crystal regime" PRL 123 197701 (2019)



Suspended CNT... isolated from the environment.



"Bottom up" fabrication.

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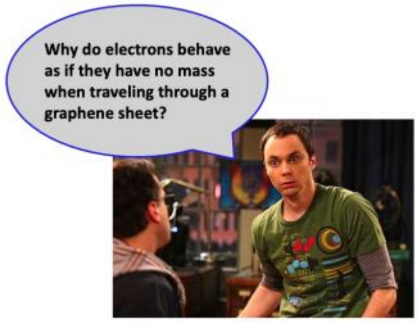
Part 2: Graphene properties

An instructive review of tight binding model from solid state physics

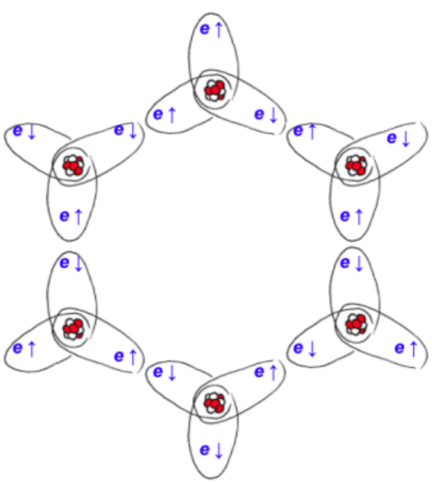
+ suprising/novel properties

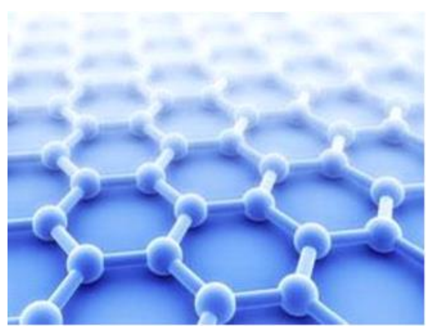


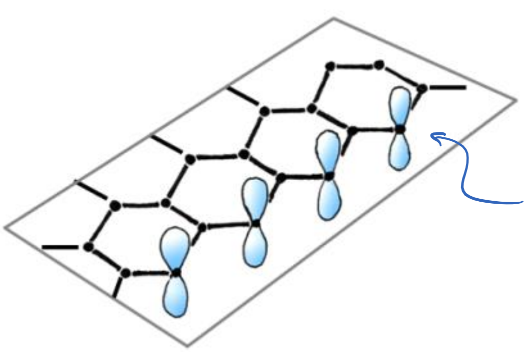
Season 3, Episode 14, "The Einstein Approximation"

Each carbon atom: 6 protons, 6 electrons

2 in core
3 participate in in-plane bonding





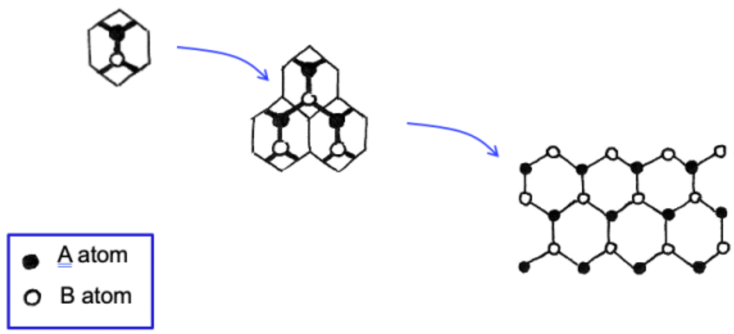


4th electron

$2p_z$ orbital

Unit cell of the crystal structure

Unit cell of the crystal structure



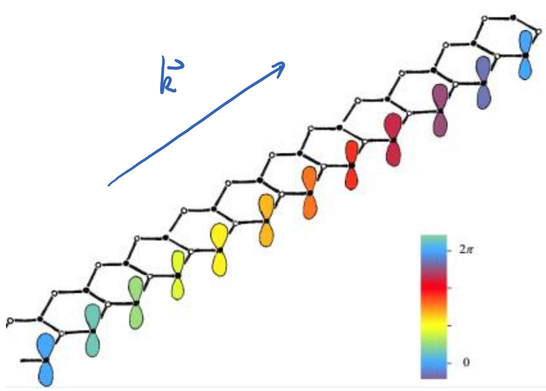
Apply Bloch theorem and use linear combination of $2p_z$ orbitals

$$\psi_{\vec{k}}(\vec{r}) = \sum_i \left(c_1^{(k)} \phi(\vec{r} - \vec{r}_{A_i}) + c_2^{(k)} \phi(\vec{r} - \vec{r}_{B_i}) \right) e^{i\vec{k}\cdot\vec{r}_i}$$

Satisfies Bloch theorem $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \underbrace{u(\vec{r})}$

$$u(\vec{r}) = u(\vec{r} + \vec{R})$$

any lattice vector



If I knew $c_1^{(\vec{k})}$ & $c_2^{(\vec{k})}$, we could already calculate

$$E_{\vec{k}} = \langle \psi_{\vec{k}}(\vec{r}) | \hat{H} | \psi_{\vec{k}}(\vec{r}) \rangle$$

$$\frac{\hat{p}^2}{2m} + V(\vec{r})$$

Instead, we have to set up a system of equations that

Instead, we have to set up a system of equations that let us solve for $c_1^{(\vec k)}$ & $c_2^{(\vec k)}$

Let the LCAO wavefunction be represented by

$$\psi_{\vec k}(\vec r) = \begin{bmatrix} c_1^{(\vec k)} \\ c_2^{(\vec k)} \end{bmatrix}$$

← first basis state

$$\psi_{\vec k}^{A}(\vec r) = \frac{1}{\sqrt N} \sum_i e^{i\vec k\cdot\vec r_{A,i}} \phi(\vec r - \vec r_{A_i})$$

second basis state

$$\psi_{k}^{B}(\vec r) = \frac{1}{\sqrt N} \sum_i e^{i\vec k\cdot\vec r_{B,i}} \phi(\vec r - \vec r_{B_i})$$

Hamiltonian when the basis set has two functions

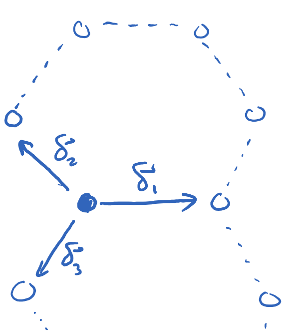
(this 2x2 matrix is now a function of $\vec k$, because basis states change with $\vec k$)

$$H_{\vec k} = \begin{bmatrix} \langle \psi_{\vec k}^{A} | H | \psi_{\vec k}^{A} \rangle & \langle \psi_{\vec k}^{B} | H | \psi_{\vec k}^{A} \rangle \\ \langle \psi_{\vec k}^{A} | H | \psi_{\vec k}^{B} \rangle & \langle \psi_{\vec k}^{B} | H | \psi_{\vec k}^{B} \rangle \end{bmatrix}$$

Note that A atoms have no A atom neighbors, so diagonal terms $= E_0$, the unperturbed energy of $2p_z$ orbital.

From now on we'll set $E_0 = 0$ (defines our reference energy).

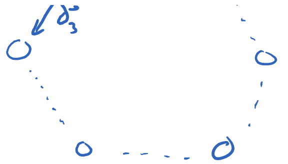
Evaluate off-diagnal elements



$$\langle \psi_B^{(k)} | H | \psi_A^{(k)} \rangle = \frac{1}{N} \int \left(\sum_i e^{i\vec k\cdot\vec r_{B,i}} \phi(r - r_{B,i}) \right)^* \hat H \left(\sum_j e^{i\vec k\cdot\vec r_{A,j}} \phi(\vec r - r_{A_j}) \right) d^3\vec r$$

for given i there are 3 values of j that give non-zero terms

$i\vec k(\vec r_{A_j} - \vec r_{B_i})$ $\quad$ $i\vec k\cdot\vec\delta_n$



that give non-zero terms

The non-zero terms will have $e^{i\vec{k}(\vec{r}_{A,i}-\vec{r}_{B,j})} = e^{i\vec{k}\cdot\vec{\delta}_\ell}$

$$= \sum_{\ell=1}^{3} e^{i\vec{k}\cdot\vec{\delta}_\ell} \underbrace{\int \phi^*(\vec{r})V(\vec{r})\,\phi(\vec{r}-\vec{\delta}_1)\,d^3\vec{r}}_{t \,\approx\, 2.7-3.0\,\mathrm{eV}}$$

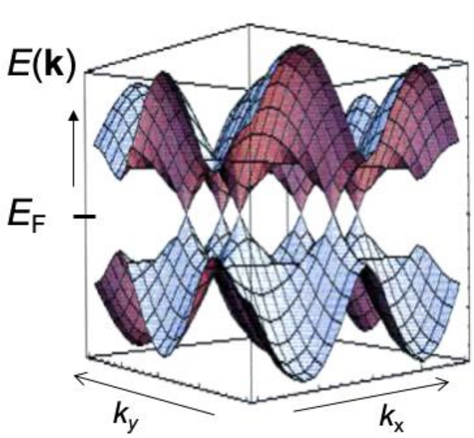
$$H_{\vec{k}} = \begin{bmatrix} 0 & \left(t\sum_{\ell=1}^{3} e^{i\vec{k}\cdot\vec{\delta}_\ell}\right) \\ \left(t\sum_{\ell=1}^{3} e^{i\vec{k}\cdot\vec{\delta}_\ell}\right)^* & 0 \end{bmatrix} = \begin{bmatrix} 0 & \Delta_k \\ \Delta_k^* & 0 \end{bmatrix}$$

$$E_{\vec{k}} = \pm\left|\Delta_{\vec{k}}\right|$$

$$\left|\sum_\ell e^{i\vec{k}\cdot\vec{\delta}_\ell}\right| = \pm\sqrt{1 + 4\cos\frac{\sqrt{3}}{2}k_y a\,\cos\frac{3}{2}k_x a + 4\cos^2\frac{\sqrt{3}}{2}k_y a}$$

Half available states in positive branch

where a is C-C bond length.



Filled states

N unit cells → 2N electrons in charge neutral graphene

→ 2N $2p_z$ orbitals

→ 4N states available. (spin up/down)

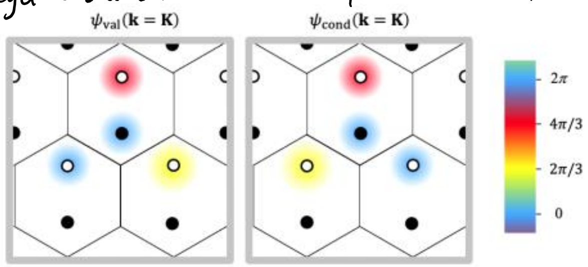
Examine wavefunction near the "Dirac point", (momentum $\vec{K}$), where valance band meets conduction band. Let $\vec{k} \simeq \vec{K}$ and look at states in the + and − branch of $\pm|\Delta_k|$.

$$\frac{1}{\sqrt{N}} \sum_i \left(c_1^{(\vec{k},\pm)} e^{i\vec{k}\cdot\vec{r}_{A,i}} \phi(\vec{r}-\vec{r}_{A,i}) + c_2^{(\vec{k},\pm)} e^{i\vec{k}\cdot\vec{r}_{B,i}} \phi(\vec{r}-\vec{r}_{B,i}) \right)$$

calculate these phase factors

mirror symmetry

negative branch   positive branch



This gives insight into the smooth cross-over from valance to conduction at E_F.

Unique states with energies that approach equal value.

To learn more about the states near the Dirac point

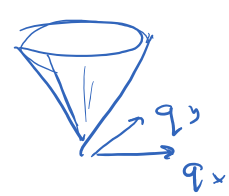
Let $\vec{k} = \vec{K} + \vec{q}$ where $|\vec{q}| \ll |\vec{k}|$

keep terms in Hamiltonian that are linear in $\vec{q}$.

$$H_{\vec{q}} = \text{const} \begin{bmatrix} 0 & q_x - i q_y \\ q_x + i q_y & 0 \end{bmatrix}$$

which has eigenvalues $E = \pm \text{const} \sqrt{q_x^2 + q_y^2}$

$$\pm \hbar v_F |\vec{q}|$$



velocity given by $\frac{1}{\hbar}\frac{dE}{dk}$

velocity given by $\frac{1}{\hbar}\frac{dE}{dk}$

v_F depends of t & a

For fun, and possible new insights, recall the Pauli spin matrices

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Then we can say

$$H_{\vec{q}} = \hbar v_F \left(q_x \hat{\sigma}_x + q_y \hat{\sigma}_y \right)$$

$$= \hbar v_F \, \vec{q} \cdot \vec{\hat{\sigma}}$$

Like the Dirac Hamiltonian for an ultrarelativistic electron

$$H = \hbar c \left(\partial_x \hat{\sigma}_x + \partial_y \hat{\sigma}_y \right)$$

speed of light

This Dirac Hamiltonian links the spin of an electron to the direction that it is traveling.

PSUEDO SPIN

For an electron in graphene, the coefficients multiplying $\psi_{\vec{k}}^{A}$ & $\psi_{\vec{k}}^{B}$ are known as the "pseudo spin".

The pseudospin is linked to the direction the electron is moving.

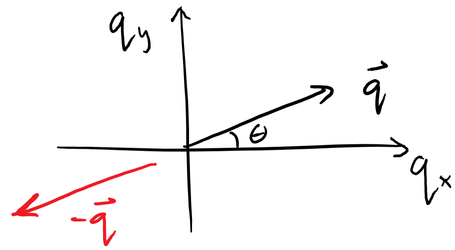
$$\begin{bmatrix} c_1^{(\vec{q})} \\ c_2^{(\vec{q})} \end{bmatrix} = \begin{bmatrix} e^{i\frac{\theta_{\vec{q}}}{2}} \\ \pm e^{-i\frac{\theta_{\vec{q}}}{2}} \end{bmatrix}$$

$$\theta_{\vec{q}} = \arctan\left(\frac{q_y}{q_x}\right)$$

$q_y \uparrow$

$$\begin{bmatrix} c_2 \end{bmatrix} \qquad \begin{bmatrix} \pm e^{\cdots} \end{bmatrix}$$

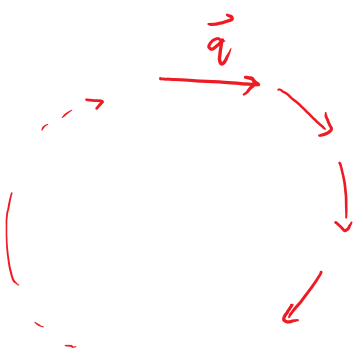
$\pm$ for states in cond / val.



Backscattering is suppressed because the pseudospins of $\vec{q}$ & $-\vec{q}$ are orthogonal to each other.

$$\begin{bmatrix} c_1^{(\vec{q})*} & c_2^{(\vec{q})*} \end{bmatrix} \begin{bmatrix} c_1^{(-\vec{q})} \\ c_2^{(-\vec{q})} \end{bmatrix} = 0$$

2 Berry's Phase



aquires Berry's phase of π after traveling in circle.

This is on top of the dynamic phase and vector potential phase.

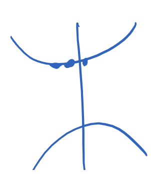
Changes the structure of Landau orbitals.

SUMMARY

Why is graphene in a class of its own.

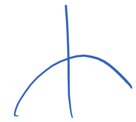
Metals: Can't tune carrier density

Semic: $E = \dfrac{p^2}{2m}$



slow moving states at band edge.

$2m$



slow moving states at band edge.

Graphene: Fast moving states at E_F $\left(\frac{c}{300}\right)$

Tune carrier density.

Unique pseudo spin property.

$\Rightarrow$ Mobility $140{,}000 \; \frac{cm^2}{V \cdot s}$ at room temp.