Two-dimensional materials and their heterostructures

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November 8th, 2016
Strong groups in:
- condensed matter,
- astrophysics,
- high energy physics

Programs!

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Outline

1. 2D materials – beyond graphene
2. Vertical heterostructures
3. Lateral heterostructures
Graphene is monolayer of carbon in honeycomb lattice.

Massless Dirac-like low energy spectrum.

Amazing physical characteristics.

Many possible applications.

Possible applications in

- Touch screens,
- photonics and plasmonics,
- RF transistors,
- lasing,
- NEMS,
- biosensing,
- flexible electronics.
A carbon atom has six electrons

- $1s$ electrons are effectively inert
- $2s$ and $2p$ electrons in different atoms can hybridize to form covalent bonds

$sp^2$ bonding gives graphene lattice

One electron per atom is left over

Can write a tight binding theory for the remaining $p_z$ electrons:

$$H = \sum_{\langle i,j \rangle} t a_i^\dagger a_j$$

Transform to reciprocal space:

$$H_k = \begin{pmatrix} 0 & t f(k) \\ t f^*(k) & 0 \end{pmatrix} \approx \begin{pmatrix} 0 & \hbar v_F (k_x + ik_y) \\ \hbar v_F (k_x - ik_y) & 0 \end{pmatrix} = \hbar v_F \sigma \cdot k$$
A smörgåsbord of 2D materials
Silicene: Graphene plus spin-orbit coupling

- Leads to quantum-anomalous Hall effect and quantum spin Hall effect

Buckling gives extra pathway:

- Easy (easier?!) integration with silicon technology

Q. Peng et al., RSC Adv. 3, 13772 (2013)

Semiconducting transition metal dichalcogenides

Strong spin-orbit coupling in the valence band gives rich spin physics
Excitons have unusually high binding energy ⇒ optoelectronic applications
Huge photoluminescence

MoS$_2$ monolayer

Picture credit: Unknown

$K$ valley

$K'$ valley

$E_F$

Fabrication of TMDs

Monolayer interfacial superconductivity:

Superconducting monolayer TMDs:

- **NbSe$_2$** becomes superconducting at $\sim 1\text{K}$


Other 2D materials

**Boron nitride**

- Insulator: Band gap $\sim 6\text{eV}$
- High quality substrate

**Phosphorene**


TI surface states

- Materials: Bi$_2$Se$_3$, Bi$_2$Te$_3$, Sb$_2$Te$_3$, and others.
- Band inversion gives ‘non-trivial’ topology
- Vacuum has ‘trivial’ topology
- 2D edge states, Dirac cones, protected by symmetry


Theory:

Experiment:
Vertical heterostructures
Vertical heterostructures

Device applications:

Transistors:

W. J. Yu et al., Nature Mater. 12, 246 (2012)

Photovoltaics:

W. J. Yu et al., Nature Nanotech. 8, 952 (2013)
Can repeat process to deposit many different layers.

Graphene on boron nitride

C. R. Dean et al., Nature 497, 598 (2013)

Complexity of the interaction

Can model moiré pattern by adding potential to Hamiltonian:

\[ V = (u_0^+ f_+ + u_0^- f_-) + \tau_z \sigma_z (u_3^+ f_- + u_3^- f_+) \]
\[ + \tau_z \sigma \cdot [l_z \times \nabla(u_1^+ f_- + u_1^- f_+)] + \Delta \tau_z \sigma_z. \]

**Physical interpretation**

<table>
<thead>
<tr>
<th>Potential modulation</th>
<th>Inversion symmetric</th>
<th>Inversion antisymmetric</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$u_0^+$</td>
<td>$u_0^-$</td>
</tr>
<tr>
<td>Modulation of hopping</td>
<td>$u_1^+$</td>
<td>$u_1^-$</td>
</tr>
<tr>
<td>Local sublattice asymmetry</td>
<td>$u_3^+$</td>
<td>$u_3^-$</td>
</tr>
<tr>
<td>Global sublattice asymmetry</td>
<td></td>
<td>$\Delta$</td>
</tr>
</tbody>
</table>

\[ u_0 = -0.15, u_1 = 0, u_3 = 0 \]
\[ u_0 = -0.108, u_1 = 0.021, u_3 = 0 \]
\[ u_0 = 0, u_1 = 0.075, u_3 = 0.075 \]
Various theoretical proposals exist for the size of the parameters:

<table>
<thead>
<tr>
<th>meV</th>
<th>$u_0^+$</th>
<th>$u_1^+$</th>
<th>$u_3^+$</th>
<th>$u_0^-$</th>
<th>$u_1^-$</th>
<th>$u_3^-$</th>
<th>$\Delta$</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model 1</td>
<td>11</td>
<td>-21</td>
<td>-18</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Point charge lattice [1]</td>
</tr>
<tr>
<td>Model 2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-11</td>
<td>-21</td>
<td>-18</td>
<td>0</td>
<td>Point charge lattice [1]</td>
</tr>
<tr>
<td>Model 3</td>
<td>1.26</td>
<td>0.7</td>
<td>-0.36</td>
<td>8.98</td>
<td>-7.31</td>
<td>-5.63</td>
<td>3.74</td>
<td>DFT [2]</td>
</tr>
<tr>
<td>Model 4</td>
<td>2</td>
<td>21</td>
<td>-0.06</td>
<td>5.2</td>
<td>-42</td>
<td>-5.9</td>
<td>5.3</td>
<td>DFT + elastic theory [3]</td>
</tr>
</tbody>
</table>

Can optical spectroscopy be a tool to determine which of these is the most realistic?


Lateral heterostructures
Fabricating lateral heterostructures


Fabricating lateral heterostructures

“Parallel stitching” method

Can grow:
- Graphene–MoS$_2$
- WS$_2$–MoS$_2$
- BN–MoS$_2$

The 2D Dirac Hamiltonian

\[ H = \hbar v_F \sigma \cdot k \]

Spectrum:

\[ E = \pm \hbar v_F k \]

Add a mass term:

\[ H = \hbar v_F \sigma \cdot k + \Delta \sigma_z \]

Spectrum:

\[ E = \pm \sqrt{(\hbar v_F k)^2 + \Delta^2} \]

Mass term caused by sublattice asymmetry, e.g. different atomic species on A and B sublattice, or perpendicular electric field for staggered lattices.
The 2D Dirac Hamiltonian with a mass term:

\[ H = \hbar v_F \sigma \cdot \mathbf{k} + \Delta \sigma_z \]

Let the mass term vary in space: \( \Delta \to \Delta(x) \)

Where \( \Delta(x) = 0 \) the gap closes and linearly dispersing (Jackiw-Rebbi) states are present.
Why is this important?

- Work by others shows Jackiw-Rebbi states in bilayer graphene
- Mass generated by perpendicular electric field
- Recent experimental verification

Qiao et al., Nano Lett. 11, 3453 (2011)

Spatially-dependent Hamiltonian:

\[ H^{\text{Sil}} = \hbar v_F (\xi \hat{k}_x \sigma_x + \hat{k}_y \sigma_y) \]
\[ + \frac{l \xi_z(x)}{2} \sigma_z + \xi_S \lambda \sigma_z \]

Silicene

\[ j_{\text{val}} = 2v + \frac{2\mu}{\hbar k_c} \]
\[ j_{\text{spin}}^{\text{TMD}} = -\frac{\lambda}{\hbar k_c} \]

D.S.L. Abergel et al.,

Spatially-dependent Hamiltonian:

\[ H^{\text{TMD}} = \hbar v_F (\xi \hat{k}_x \sigma_x + \hat{k}_y \sigma_y) \]
\[ + \frac{\Delta(x)}{2} \sigma_z - \xi_S \lambda \frac{\sigma_z - \sigma_0}{2} \]

D.S.L. Abergel et al.,
2D Heterostructures
The BN on either side can be in two topological configurations.
- Either the boron is on the A sublattice, or the nitrogen is.
- If the topologies are “opposite” the graphene hosts gapless modes.
- If the two topologies are the “same” then there is no guarantee of low energy modes.

Growth imperfections

Growth of lateral heterostructures is not perfectly controlled.

Graphene – boron nitride

Transition metal dichalcogenides


X. Duan et al., Nature Nanotech. 9, 1024 (2014).

P. Sutter et al., Nano Lett. 12, 4869 (2012).

Some subtlety:

- Strictly speaking the topological protection is only *per valley*.
- Lattice scale disorder can couple valleys, *break protection*.
- CVD techniques to not produce perfect interfaces.

The question is, how robust are desirable properties related to these modes against lattice scale disorder?

- Tight binding model.
- Scattering theory plus Landauer formula for conductance.
- Compute conductance for 200 disorder manifestations
- $\theta$ is variance of distribution of angular deflections
- Take mean conductance at each energy value
- Extract fifth percentile conductance at each energy value

Summary

- 2D materials show massive additional functionality when combined into heterostructures.
- Inversion of Dirac mass leads to topologically protected valley and spin currents with spin-orbit coupling.
- Transport in BN–graphene–BN wires highly robust as long as armchair edges and vacancies are minimised.
- (Strong modification of nearest-neighbour hopping by BN substrate can be detected in absorption spectroscopy.)

Slides available at: bit.ly/AbergelTalks

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References:
What’s going on? Edge types

What's going on? Edge types

AC protrusion
No protrusion

What’s going on? Topological interpretation

- Atomic substitution is ‘adiabatic’
- Carbon vacancy is new topology

**Summary:**
- Zigzag edges and atomic substitutions **do not** couple valleys
  \[ \Rightarrow \text{topological protection works} \]
- Armchair edges and atomic vacancies **do** couple valleys
  \[ \Rightarrow \text{topological protection does not work} \]