Gap induction in single and bilayer graphene

MMM, 23.11.2009

Dorothée Hug
Outline

• Single layer graphene
• Energy gaps in graphene nanoribbons (GNR)  
  – Son et al., PRL 97, 216803, 2006
• Band gap engineering in GNR  
  – Han et al., PRL 98, 206805, 2007
• Coulomb blockade in GNR  
  – Sols et al., PRL 99, 166803, 2007
• Gate-induced insulating states in BLG devices  
  – Oostinga et al., nature materials, doi:10.1038/mat2082
• Conclusion
Graphene

No band gap in intrinsic graphene! Confinement should lead to an induction of a band gap!

M. Wilson, Physics Today, 21, 2006
Energy gaps in graphene nanoribbons

First principle calculation of bandstructure for graphene ribbons with hydrogen passivated armchair or zigzag edges
Band gap for GNR with ideal edges

\[ \delta a_n \equiv 100 \times \frac{a_n - a_c}{a_c} \]

3.3-3.5\% decrease in bonding length leads to 12\% increase in hopping integral between \( \pi \)-orbitals
Band gap for GNR with ideal edges

\[ \mathcal{H} = \sum_{n=1}^{N_a} \sum_{\mu=1}^{2} \varepsilon_{\mu,n} a_{\mu,n}^{\dagger} a_{\mu,n} \\
- \sum_{n=1}^{N_a} t_n^{\parallel} (a_{1,n}^{\dagger} a_{2,n} + \text{H.c.}) \\
- \sum_{n=1}^{N_a-1} \sum_{\mu=1}^{2} t_{n,n+1}^{\parallel} (a_{\mu,n}^{\dagger} a_{\mu,n+1} + \text{H.c.}) \]

\[ \Delta_{3p} > \Delta_{3p+1} > \Delta_{3p+2} > 0 \]
Energy gaps in zigzag ribbons

\[ \Delta_z^0, \Delta_z^1 \]

\[ 0, \pi \]

\[ E - E_F (eV) \]

\[ k(1/d_z) \]

\[ \Delta_z^0 \]

\[ \Delta_z^1 \]

\[ w_z(\text{Å}) \]

\[ \Delta_z (eV) \]
Energy band gap engineering of GNR
Width dependence of the conductance

\[ G = \sigma(W - W_0)/L \]

- **W-W0**: active transport width of the ribbon
- **\( \sigma \)**: Conductivity of the ribbon
Direct measurement of the gap in GNR
Dependence of $E_{\text{gap}}$ on the ribbon width

**Experimental**

$E_g = \alpha / (W - W_0)$

$G = \beta (W - W_0)$

$W_0 \approx 16\text{nm}$ at 1.6K

gap size $> 0.1$-$0.2\text{eV}$

**Theoretical**

No interaction effects:

$E_g = \hbar v_f / (W 2\pi)$

with $v_f = 10^6 \text{m/s}$

gap size $< 0.2\text{eV}$

Differences could be due to:

a) Overestimation of ribbon width

b) Reduction of effective transport width due to disorder at edges

c) Coulomb blockade effects
Coulomb blockade in GNR

Energy level spacing of delocalized states in a region of size $W$:

$$E_g \approx \frac{\hbar v_F}{W}$$

Charging energy of a dot of size $W$:

$$E_c \sim \frac{e^2}{W}$$

Conductance for small average transmission per channel:

$$G \approx (4G_Qk_F\tau/\pi)(W - W_0)$$

$\longrightarrow \tau \approx 0.07$
Inducing band gaps in bilayer graphene

$$\psi = \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix}$$

$$H = \begin{pmatrix} \Delta & \hbar v_F (k_x - ik_y) \\ \hbar v_F (k_x + ik_y) & -\Delta \end{pmatrix}$$

$$E = \pm \hbar v_F |k|$$

$$E = \pm \hbar^2 k^2 / 2m$$

$$H = \begin{pmatrix} \Delta & -\frac{\hbar^2}{2m} (k_x - ik_y)^2 \\ -\frac{\hbar^2}{2m} (k_x + ik_y)^2 & -\Delta \end{pmatrix}$$

23.11.2009

Oostinga et al., nature materials, doi:10.1038/mat2082
Inducing band gaps in bilayer graphene
Conclusion

• ACGNR and ZGNR show a band gap in theory, which is dependent on $1/W$
• Experiments measured a gap with $1/W$ dependence
• It is not clear if the gap is due to band gap opening or reduction of current through the ribbon
• Inducing band gaps in BLG can be done by applying a electric field