Introduction
Main properties
The need of a band-gap
Opening a bandgap
Why graphene is gapless?
Designing semiconducting structures
Summary

Symmetry-induced band-gap opening in graphene superlattices

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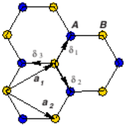
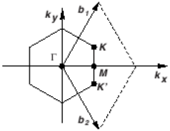
Basic electronic structure

$$H \approx -t \sum_{i,\tau} \sum_j a^\dagger_\tau(\mathbf{R}_i) b_\tau(\mathbf{R}_i + \delta_j) + c.c.$$

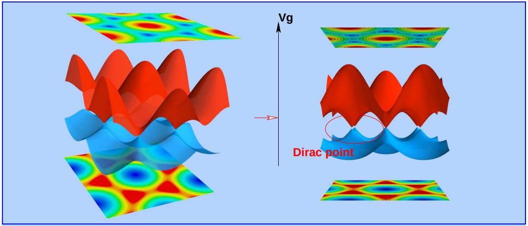


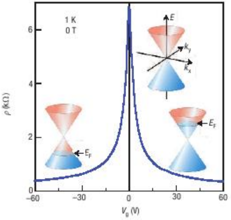


$$a_{\tau;i} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{R}_i} a_\tau(\mathbf{k})$$

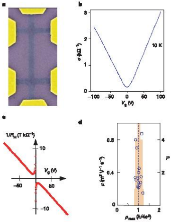
$$H = -t \sum_{\mathbf{k},\tau} f(\mathbf{k}) a^\dagger_\tau(\mathbf{k}) b_\tau(\mathbf{k}) + c.c.$$

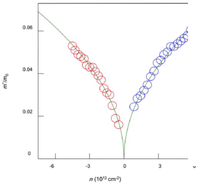
$$H = -t \sum_{\mathbf{k},\tau} \left[a^\dagger_\tau(\mathbf{k}), b^\dagger_\tau(\mathbf{k}) \right] \begin{bmatrix} 0 & f(\mathbf{k}) \\ f^*(\mathbf{k}) & 0 \end{bmatrix} \begin{bmatrix} a_\tau(\mathbf{k}) \\ b_\tau(\mathbf{k}) \end{bmatrix}$$

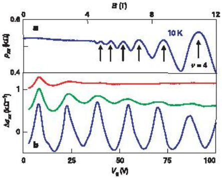


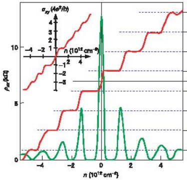


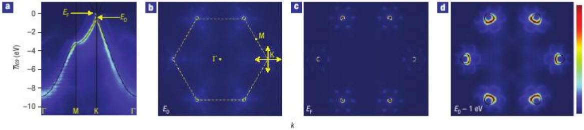
Basic electronic structure

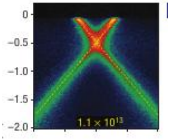












Device related properties

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- **Thickness**: thinnest gate-controlled regions in transistors
- **Mobility**: high-mobility carriers
- **High-field transport**: high saturation velocities
- **Band-gap**: high on-off ratios are not achievable without a bandgap

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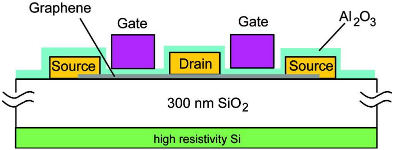
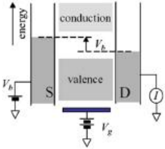
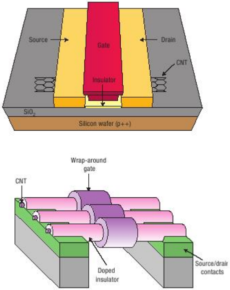
Logic applications



$$n_S = \epsilon_0 \epsilon \frac{V_g}{t\,e}$$





CNT-FET with ordinary and wrapped around gates

P. Avouris *et al.*, *Nat. Mat.*, 605, 2, (2007)

F. Schwiertz, *Nat. Nanotech.* **5**, 487 (2010)

Logic applications

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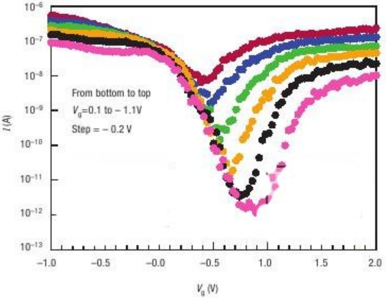
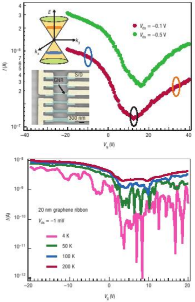


$I - V_g$ characteristics of a CNT-FET



$I = I(V_g, V_{ds})$ GNR-FET

Band-gap opening

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- **Electron confinement**: nanoribbons, (nanotubes),etc.
- **Symmetry breaking**: epitaxial growth, deposition, etc.
- **Symmetry preserving**: “supergraphenes”

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e-*h* symmetry

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$$H^{TB} = \sum_{\sigma,ij}(t_{ij} a^{\dagger}_{i,\sigma} b_{j,\sigma} + t_{ji} b^{\dagger}_{j,\sigma} a_{i,\sigma})$$

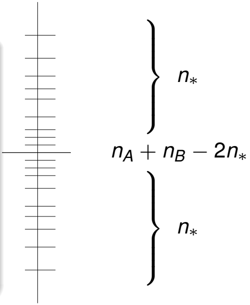
Electron-hole symmetry

$$b_i \rightarrow -b_i \Longrightarrow \mathbf{h} \rightarrow -\mathbf{h}$$

if ϵ_i is eigenvalue and
$c_i^{\dagger} = \sum_i \alpha_i a_i^{\dagger} + \sum_j \beta_j b_j^{\dagger}$ eigenvector

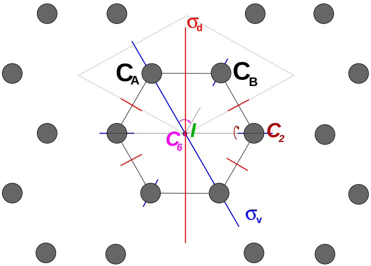
$$\Downarrow$$

$-\epsilon_i$ is also eigenvalue and
$c_i^{\prime\,\dagger} = \sum_i \alpha_i a_i^{\dagger} - \sum_j \beta_j b_j^{\dagger}$ is eigenvector



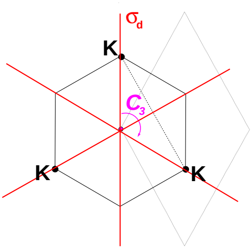
Spatial symmetry

r-space



$G_0 = D_{6h}$

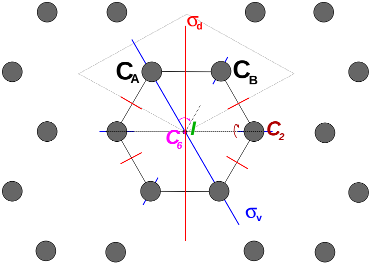
k-space



$G(\mathbf{k}) = \{g \in G_0 | g\mathbf{k} = \mathbf{k} + \mathbf{G}\}$
$\Rightarrow G(\mathbf{K}) = D_{3h}$

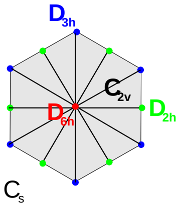
Spatial symmetry

***r*-space**



$$G_0 = D_{6h}$$

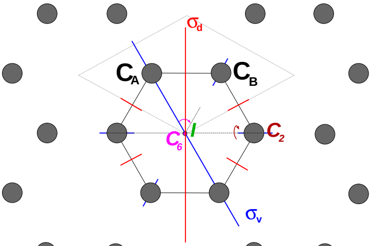
***k*-space**



$$G(\mathbf{k}) = \{g \in G_0 | g\mathbf{k} = \mathbf{k} + \mathbf{G}\}$$
$$\Rightarrow G(\mathbf{K}) = D_{3h}$$

Spatial symmetry

***r*-space**



$G_0 = D_{6h}$

$$|A_{\mathbf{k}}\rangle = \frac{1}{\sqrt{N_{BK}}} \sum_{\mathbf{R}\in BK} e^{-i\mathbf{kR}} |A_{\mathbf{R}}\rangle$$

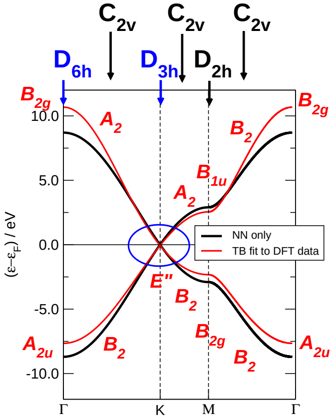
$$|B_{\mathbf{k}}\rangle = \frac{1}{\sqrt{N_{BK}}} \sum_{\mathbf{R}\in BK} e^{-i\mathbf{kR}} |B_{\mathbf{R}}\rangle$$

$$\langle r|A_{\mathbf{R}}\rangle = \phi_{p_Z}(\mathbf{r}-\mathbf{R})$$

for $\mathbf{k} = \mathbf{K}$

$\{|A_{\mathbf{k}}\rangle, |B_{\mathbf{k}}\rangle\}$ span the E'' irrep of D_{3h}

Spatial symmetry



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for $\mathbf{k} = \mathbf{K}$

$\{|A_{\mathbf{k}}\rangle, |B_{\mathbf{k}}\rangle\}$ span the E'' irrep of D_{3h}

Spatial and *e-h* symmetry

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Lemma

e-h symmetry holds within each kind of symmetry species (A, E, ..)

Theorem

For any bipartite lattice at half-filling, if the number of E irreps is odd at a special point, there is a degeneracy at the Fermi level, i.e. $E_{gap} = 0$

A simple recipe

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- Consider *nxn* graphene superlattices (i.e. $G = D_{6h}$): degeneracy is expected at Γ, K
- Introduce p_z vacancies while preserving point symmetry
- Check whether it is possible to turn the number of E irreps to be even both at Γ and at K

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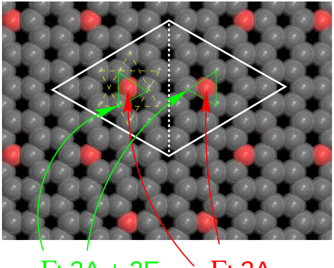
Counting the number of E irreps

$$n = 4$$



Γ: 2A + 2E
K: 2A + 2E

Γ: 2A
K: E

Γ	A	E
$\bar{0}_3$	$2m^2$	$2m^2$
$\bar{1}_3$	$2(3m^2+2m+1)$	$2(3m^2+2m)$
$\bar{2}_3$	$2(3m^2+4m+2)$	$2(3m^2+4m+1)$
K_n	A	E
$\bar{0}_3$	$2m^2$	$2m^2$
$\bar{1}_3$	$2m(3m+2)$	$2m(3m+2)+1$
$\bar{2}_3$	$2(3m^2+4m+1)$	$2(3m^2+4m+1)+1$

$$\Rightarrow n = 3m+1, 3m+2,\ m \in \mathbb{N}$$

An example

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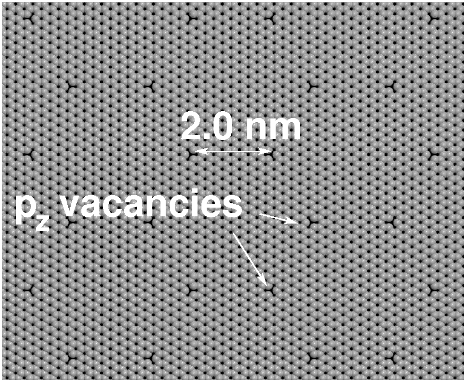
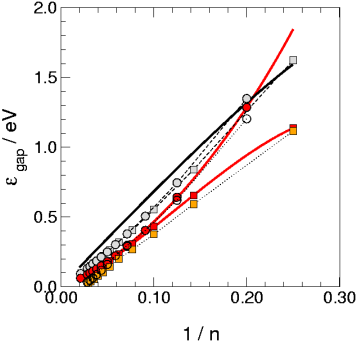
$(14, 0)$-honeycomb



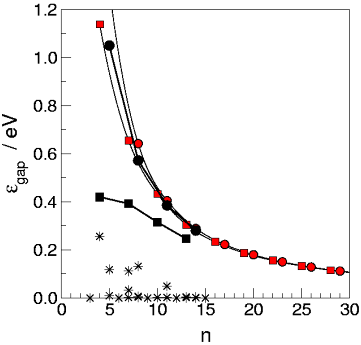
Band-gap opening..

Tight-binding



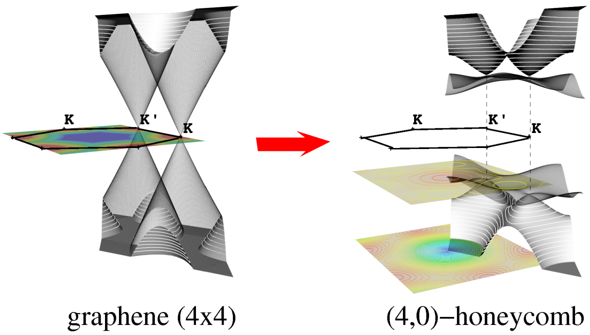
$$\epsilon_{gap}(K) \sim 2t\sqrt{1.683}/n$$

DFT



..and Dirac cones

..not only: as degeneracy may still occur at $\epsilon \neq \epsilon_F$
new Dirac points are expected



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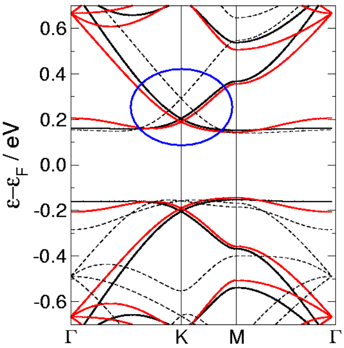
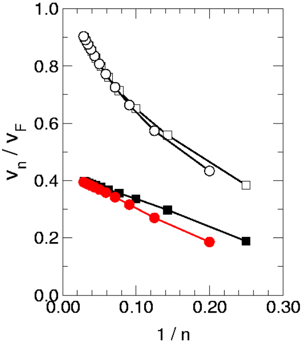
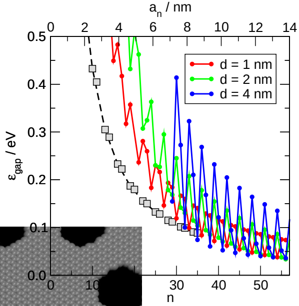
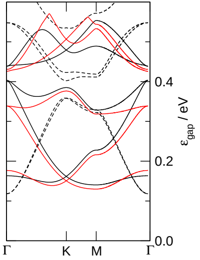


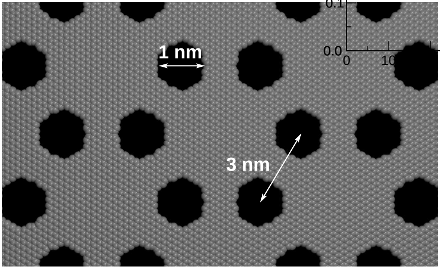


Antidot superlattices

...the same holds for honeycomb antidots







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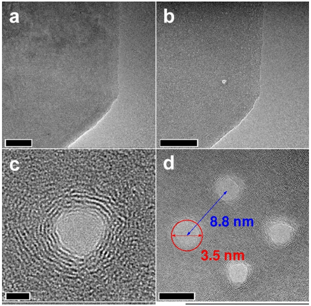
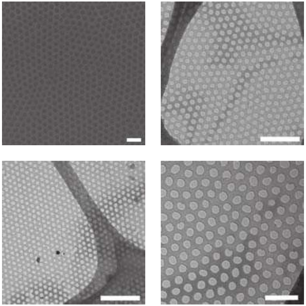


M. D. Fishbein and M. Drndic, *Appl. Phys. Lett.* **93**, 113107 (2008)
T. Shen *et al. Appl. Phys. Lett.* **93**, 122102 (2008)



J. Bai *et al. Nature Nantotech.* **5**, 190 (2010)

..novel transistor?

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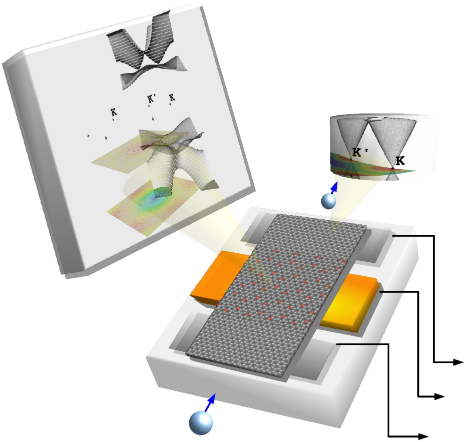

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- Symmetry *breaking* is not necessary to open a gap
- New Dirac cones appears right close to the edges of the gap region
- Honeycomb antidot superlattices should be experimentally feasible

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Thanks for your attention!