Spin-orbit interaction in graphene, nanotubes, fullerenes

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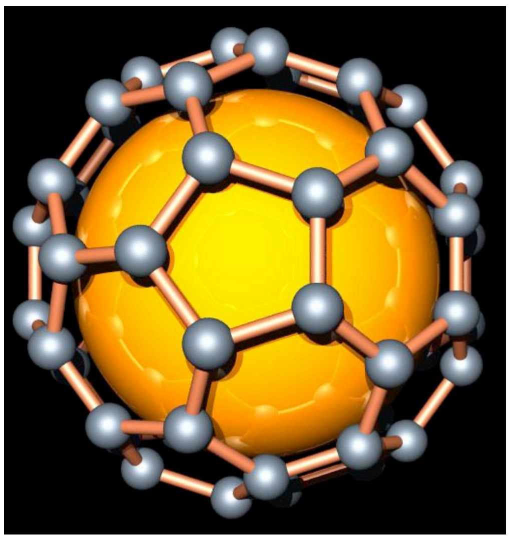
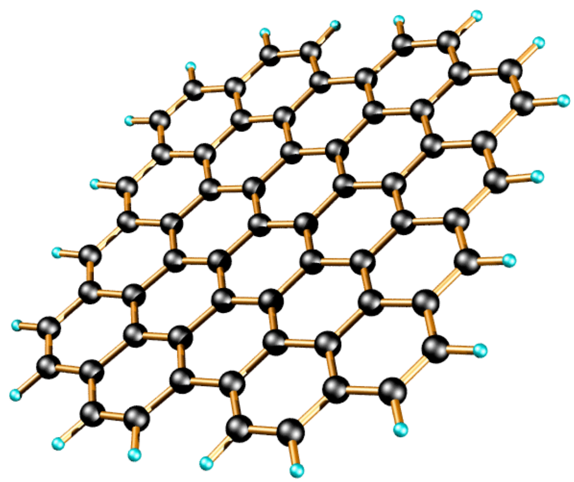
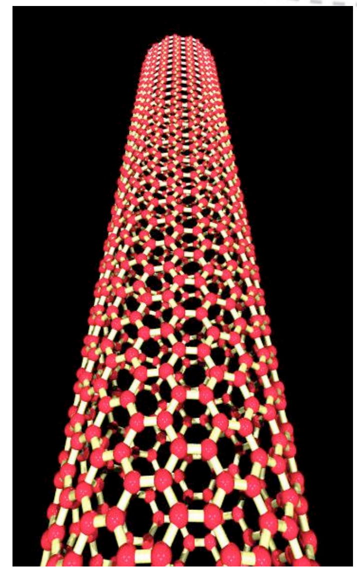
Phys. Rev. B **74**, …(2006) in print; cond-mat/0606580.







Graphene week-MPI PKS Dresden
September 25-29

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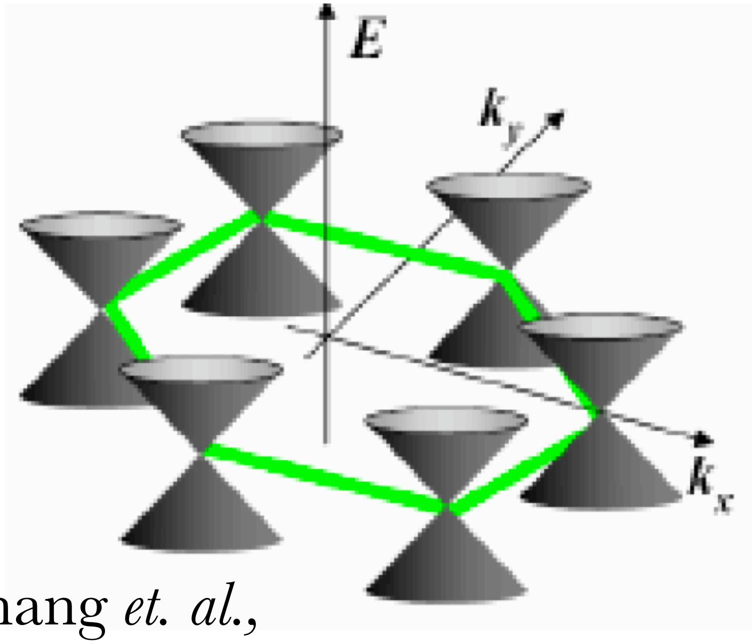
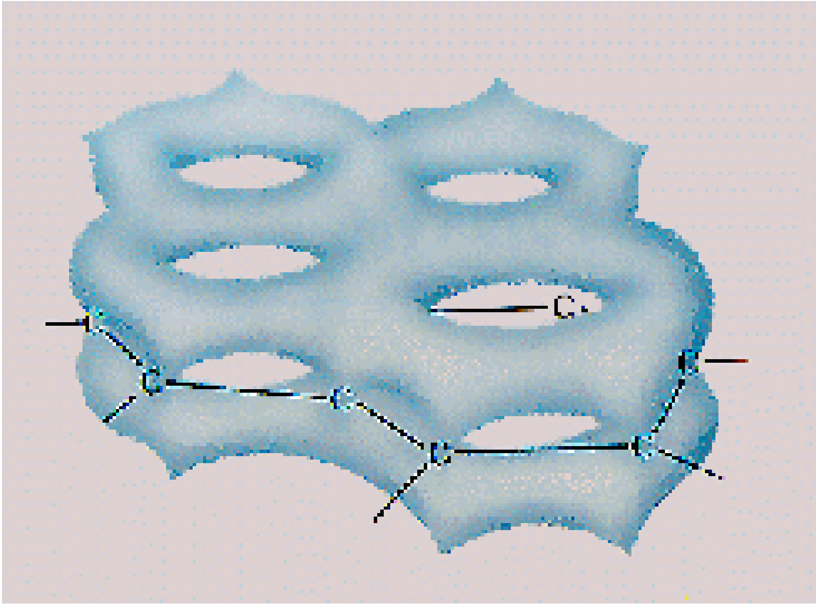


Fig.
Y.Zhang *et. al.*,
Nature **438**,
201-204, (2005)



$$H = \Psi^\dagger \left(-i\,\vec{\gamma}\cdot\vec{\nabla}\right)\Psi$$

$$\vec{\gamma} = \hbar v_F\left(\hat{\sigma}_x, \hat{\tau}_z\hat{\sigma}_y\right);\ \hbar v_F = \frac{\sqrt{3}\gamma_o a}{2} \sim 5.3\ \text{eV Å}$$

$$\hat{\sigma} - A, B\ sublattice \qquad a \sim 2.46\,\text{Å}$$

$$\hat{\tau} - K, K' \qquad \gamma_o \sim 3\text{eV}$$

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Is S-O important in graphene?:

- Atomic Spin-Orbit is supposed to be rather weak in Carbon as Z=6:
    - Is S-O in graphene small?: YES. How small and why!!!
    - Spin Quantum Hall effect proposal by Kane&Mele.
- Controlling pseudo-spin by means of coupling to the spin!
- Spintronics in graphene:
    - Spin-flip due to S-O. How important ?
- Induced Ferromagnetism in proton irradiated samples.

[P. Esquinazi *et. al.*,PRL **91**, 227201 (2003)]

…..??

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Atomic spin orbit

$$\mathcal{H}_{\mathrm{SO}} = \Delta \tilde{\mathbf{L}} \tilde{\mathbf{s}}$$

$$\mathcal{H}_{\mathrm{SO}} = \Delta \left[\frac{L_+ s_- + L_- s_+}{2} + L_z s_z \right]$$

$$|p_z\rangle \equiv |L = 1, L_z = 0\rangle$$ π−bands

$$|p_x\rangle \equiv \frac{1}{\sqrt{2}} \left(|L = 1, L_z = 1\rangle + |L = 1, L_z = -1\rangle \right)$$

$$|p_y\rangle \equiv \frac{-i}{\sqrt{2}} \left(|L = 1, L_z = 1\rangle - |L = 1, L_z = -1\rangle \right)$$

σ−bands

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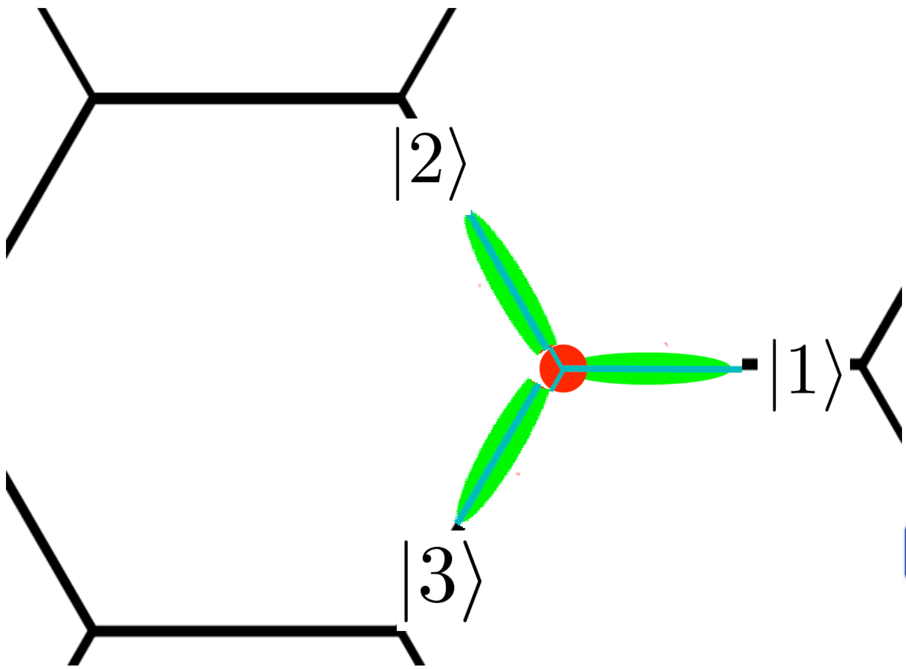
The sigma σ bands: sp^2 hybridization

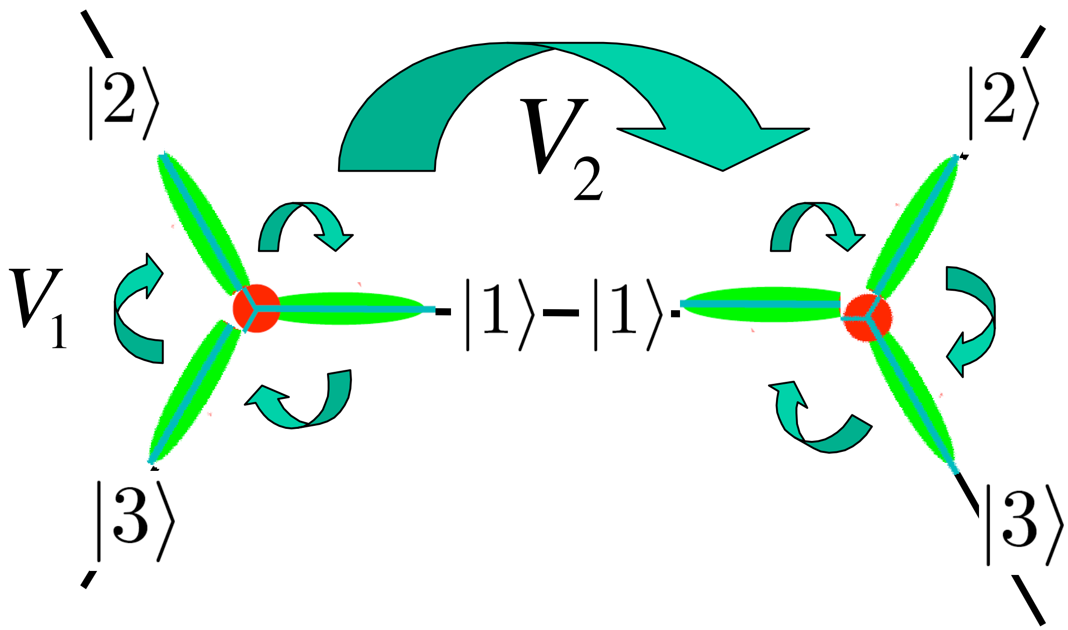
$$
\begin{aligned}
|1\rangle &\equiv \frac{1}{\sqrt{3}}\left(|s\rangle + \sqrt{2}|p_x\rangle\right) \\
|2\rangle &\equiv \frac{1}{\sqrt{3}}\left[|s\rangle + \sqrt{2}\left(-\frac{1}{2}|p_x\rangle + \frac{\sqrt{3}}{2}|p_y\rangle\right)\right] \\
|3\rangle &\equiv \frac{1}{\sqrt{3}}\left[|s\rangle + \sqrt{2}\left(-\frac{1}{2}|p_x\rangle - \frac{\sqrt{3}}{2}|p_y\rangle\right)\right]
\end{aligned}
$$

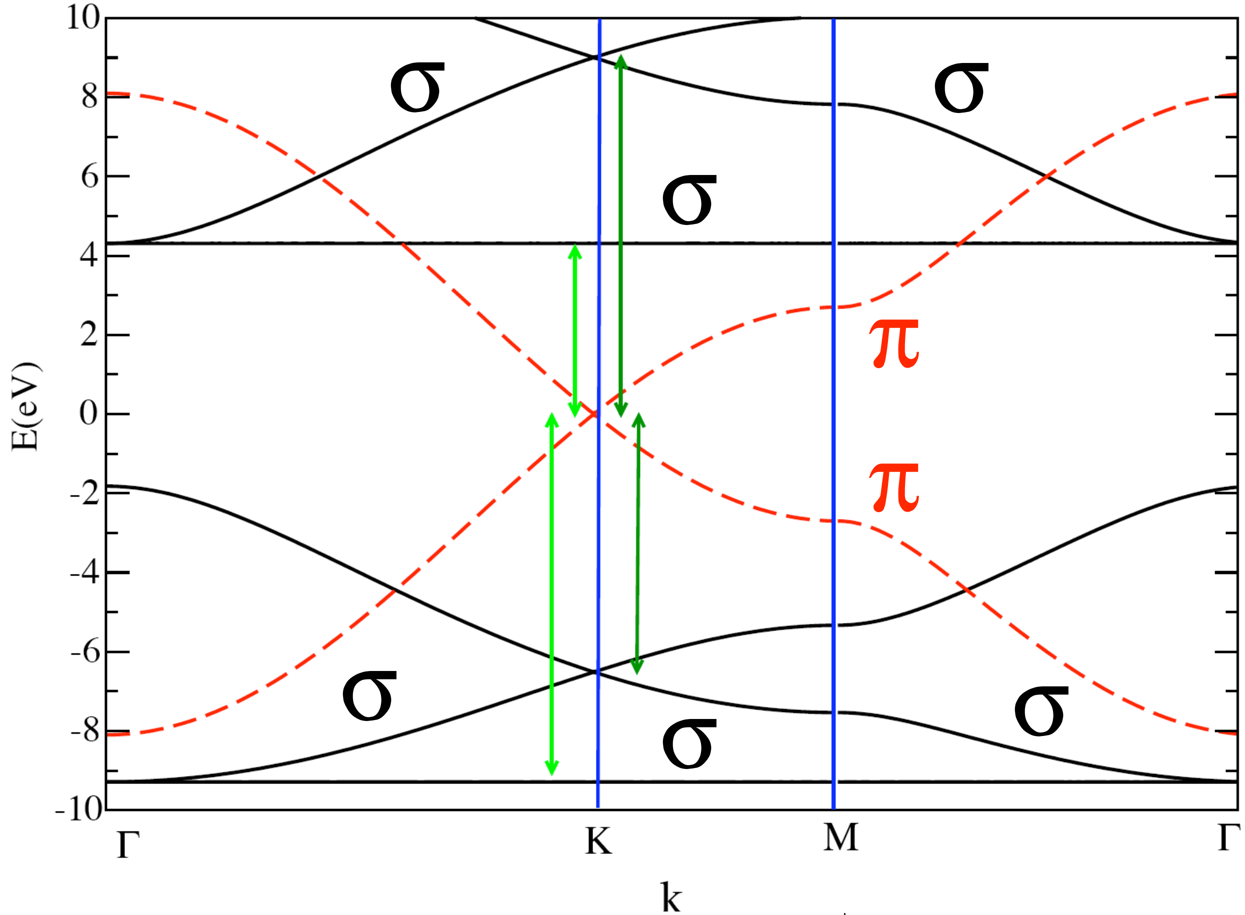


M. F. Thorpe and D. Weaire, Phys. Rev. Lett. **27**, 1581 (1971)

$$\mathcal{H}_\sigma = V_1 \sum_{\substack{\alpha\neq\beta \\ i}} c^\dagger_{i\alpha} c_{i\beta} + V_2 \sum_{\substack{<i,j> \\ \alpha,\alpha'}} c^\dagger_{i\alpha} c_{j\alpha'} + h.c.$$

$$V_1 = \frac{\epsilon_s - \epsilon_p}{3} \qquad V_2 = \frac{V_{ss\sigma} + 2\sqrt{2}V_{sp\sigma} + 2V_{pp\sigma}}{3}$$





two σ Dirac spinors $\psi_{\sigma 1}$ $\psi_{\sigma 2}$

$$\epsilon_\sigma(\mathbf{k}) = \frac{V_1}{2} \pm \sqrt{\frac{9}{4}V_1^2 + V_2^2 \pm V_1 V_2 f(\mathbf{k})}.$$

two other "flat" orbitals $\phi_{\sigma 1}$ $\phi_{\sigma 2}$

$$\epsilon_\sigma(\mathbf{k}) = -V_1 \pm V_2$$

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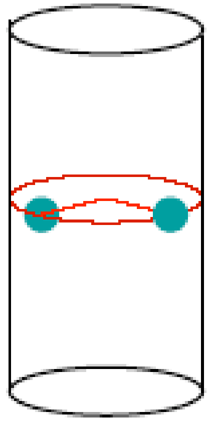
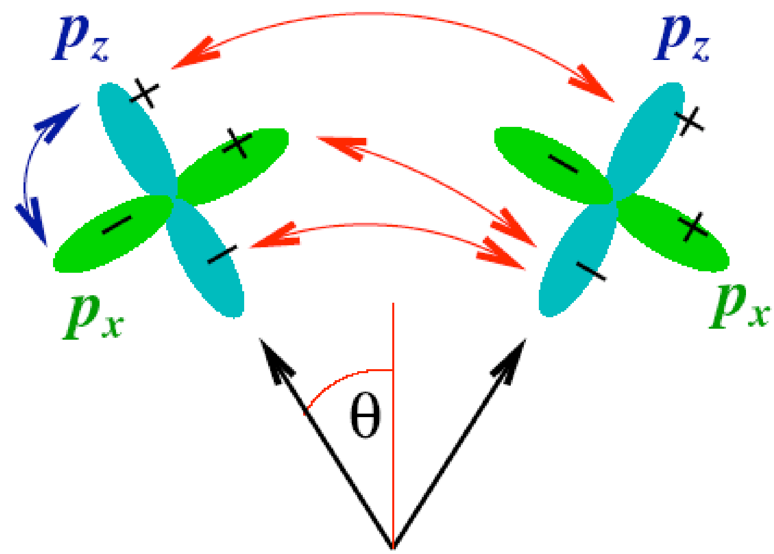
Curvature





$$\mathcal{H} = \mathcal{H}_{\mathrm{SO1}} + \mathcal{H}_{\mathrm{SO2}} + \mathcal{H}_{\mathrm{ion1}} + \mathcal{H}_{\mathrm{ion2}} + \mathcal{H}_{\mathrm{T}}$$

$$\mathcal{H}_{\mathrm{SOi}} = \Delta \left[c^\dagger_{zi\uparrow} c_{xi\downarrow} + c^\dagger_{zi\downarrow} c_{xi\uparrow} \right] + h.c.$$

$$\mathcal{H}_{\mathrm{ioni}} = \epsilon_\pi \sum_s c^\dagger_{zis} c_{zis} + \epsilon_\sigma \sum_s c^\dagger_{xis} c_{xis}$$

$$\mathcal{H}_{\mathrm{T}} = \sum_s \left[V_\pi \cos^2(\theta) + V_\sigma \sin^2(\theta) \right] c^\dagger_{z1s} c_{z0s} - \left[V_\pi \sin^2(\theta) + V_\sigma \cos^2(\theta) \right] c^\dagger_{x1s} c_{x0s} +$$

$$+ \sin(\theta)\cos(\theta)\,(V_\pi - V_\sigma) \left(c^\dagger_{z1s} c_{x0s} - c^\dagger_{x1s} c_{z0s} \right) + h.c.$$

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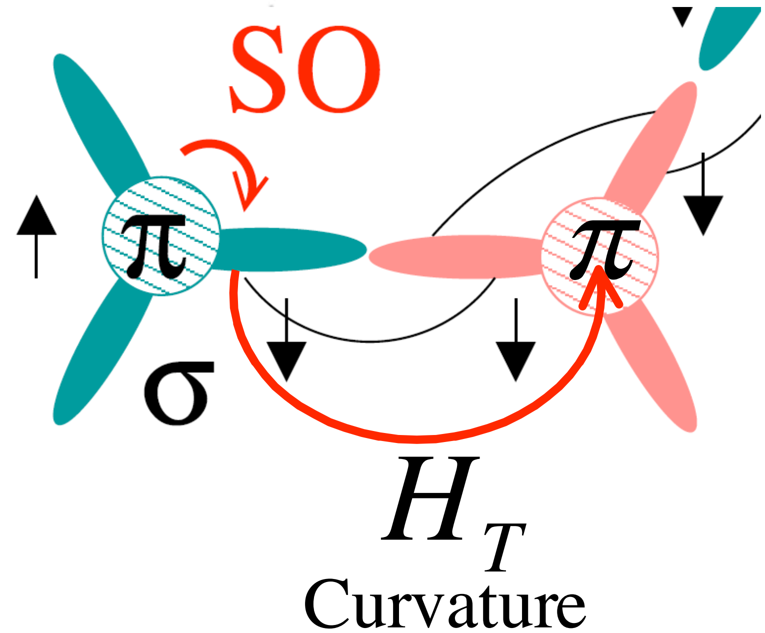
Atomic spin-orbit Δ+hopping σ−π

$$|p_z 0 \uparrow\rangle \xrightarrow{\;\Delta\;} |p_x 0 \downarrow\rangle \xrightarrow{\mathcal{H}_\mathrm{T}} |p_z 1 \downarrow\rangle$$

$$|p_z 0 \uparrow\rangle \xrightarrow{\mathcal{H}_\mathrm{T}} |p_x 0 \uparrow\rangle \xrightarrow{\;\Delta\;} |p_z 1 \downarrow\rangle$$



$$\mathcal{H}_\mathrm{T} = \sin(\theta)\cos(\theta)\left(V_{pp\pi} - V_{pp\sigma}\right)\left(c^\dagger_{z1s'}c_{x0s'} - c^\dagger_{x1s'}c_{z0s'}\right) + h.c.$$

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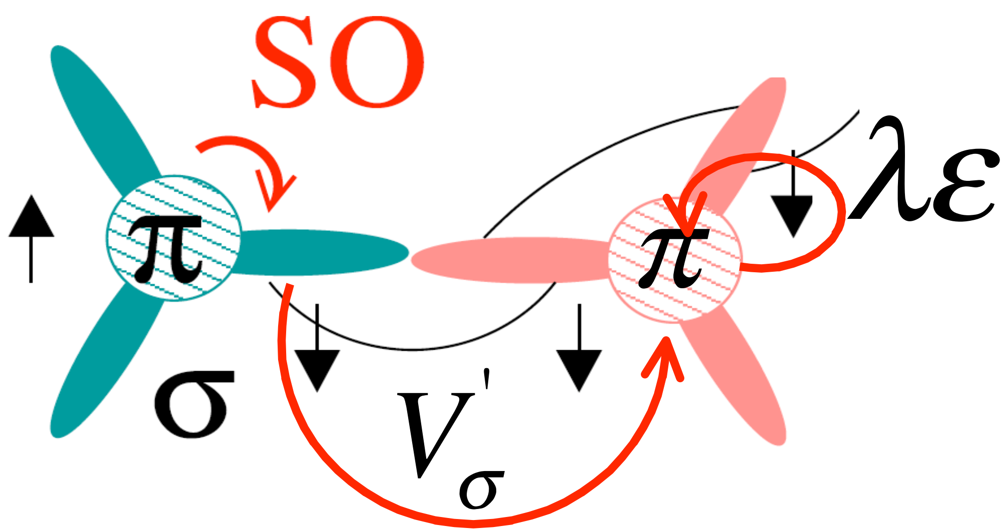
Atomic spin-orbit Δ +hopping σ−π

$$|p_z 0\uparrow\rangle \xrightarrow{\lambda\mathcal{E}} |s0\uparrow\rangle \xrightarrow{V'_\sigma} |p_x 1\uparrow\rangle \xrightarrow{\Delta} |p_z 1\downarrow\rangle$$

$$|p_z 0\uparrow\rangle \xrightarrow{\Delta} |p_x 0\downarrow\rangle \xrightarrow{V'_\sigma} |s1\downarrow\rangle \xrightarrow{\lambda\mathcal{E}} |p_z 1\downarrow\rangle$$



$$\lambda \equiv \langle p_z | \hat{z} | s \rangle$$

Electric dipole transition

Atomic Stark effect

Atomic spin-orbit Δ^2 +hopping σ

V_σ :

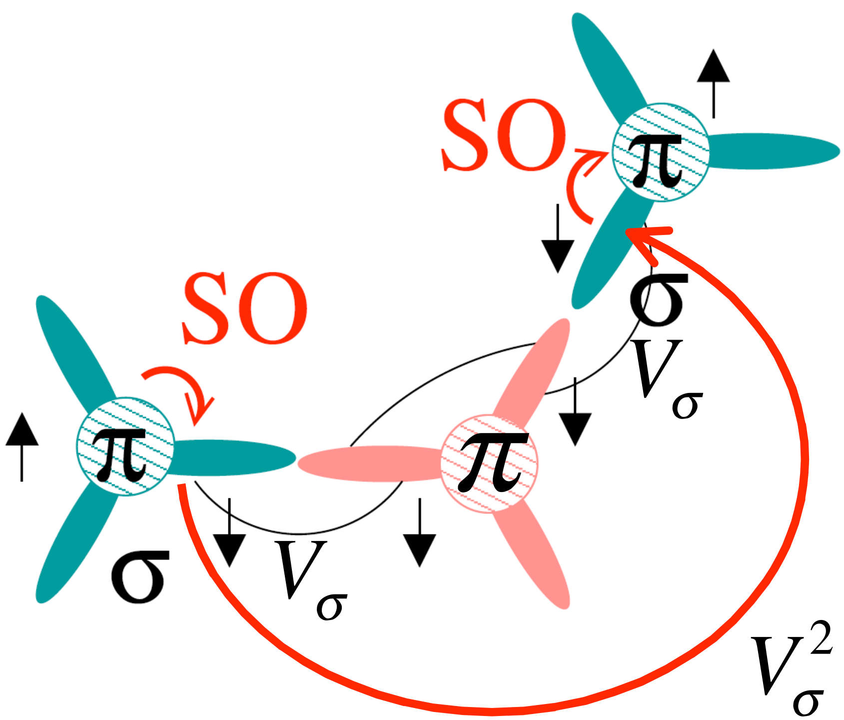
$$|p_z 0\uparrow\rangle \xrightarrow{\Delta} |p_x 0\downarrow\rangle \xrightarrow{V_\sigma} |p_x 1\downarrow\rangle \xrightarrow{\Delta} |p_z 1\uparrow\rangle$$

$$|p_z 0\uparrow\rangle \xrightarrow{\Delta} -\tfrac{1}{2}|p_x 0\downarrow\rangle + \tfrac{\sqrt{3}}{2}|p_y 0\downarrow\rangle \xrightarrow{V_\sigma} \tfrac{1}{2}|p_x 2\downarrow\rangle - \tfrac{\sqrt{3}}{2}|p_y 2\downarrow\rangle \xrightarrow{\Delta} |p_z 2\uparrow\rangle$$

$$|p_z 0\uparrow\rangle \xrightarrow{\Delta} -\tfrac{1}{2}|p_x 0\downarrow\rangle - \tfrac{\sqrt{3}}{2}|p_y 0\downarrow\rangle \xrightarrow{V_\sigma} \tfrac{1}{2}|p_x 3\downarrow\rangle + \tfrac{\sqrt{3}}{2}|p_y 3\downarrow\rangle \xrightarrow{\Delta} |p_z 3\uparrow\rangle$$

=0!!!

V_σ^2 :....



Atomic spin-orbit Δ process bewteen π and σ

$$\mathcal{H}_{SOK} \equiv \frac{\Delta}{2}\int d^2\vec{\mathbf{r}}\sqrt{\frac{2}{3}}\left\{\cos\left(\frac{\alpha}{2}\right)\left[\Psi^\dagger_{AK\uparrow}(\vec{\mathbf{r}})\psi_{\sigma 1AK\downarrow}(\vec{\mathbf{r}}) + \Psi^\dagger_{BK\uparrow}(\vec{\mathbf{r}})\psi_{\sigma 1BK\downarrow}(\vec{\mathbf{r}})\right] + \sin\left(\frac{\alpha}{2}\right)\left[\Psi^\dagger_{AK\uparrow}(\vec{\mathbf{r}})\psi_{\sigma 2AK\downarrow}(\vec{\mathbf{r}}) + \Psi^\dagger_{BK\uparrow}(\vec{\mathbf{r}})\psi_{\sigma 2BK\downarrow}(\vec{\mathbf{r}})\right]\right\} + \sqrt{\frac{2}{3}}\left[\Psi^\dagger_{AK\uparrow}(\vec{\mathbf{r}}) + \Psi^\dagger_{BK\uparrow}(\vec{\mathbf{r}})\right]\phi_{1\downarrow}(\vec{\mathbf{r}}) + h.c.$$

$$\alpha = \arctan\left[\frac{(3V_1)/2}{\sqrt{(9V_1^2)/4 + V_2^2}}\right].$$

Similar expression for K'

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Effective Hamiltonian

Order Δ

$$\mathcal{H}_{\mathrm{curv}K\pi} \equiv -i\frac{\Delta(V_{pp\sigma}-V_{pp\pi})V_1}{2V_1^2+V_2^2}\left(\frac{a}{R_1}+\frac{a}{R_2}\right)\int d^2\vec{\mathbf{r}}\left(\Psi^\dagger_{AK\uparrow}(\vec{\mathbf{r}})\Psi_{BK\downarrow}(\vec{\mathbf{r}})-\Psi^\dagger_{BK\downarrow}\Psi_{AK\uparrow}\right).$$

$$\mathcal{H}_{\mathrm{curv}K'\pi} \equiv -i\frac{\Delta(V_{pp\sigma}-V_{pp\pi})V_1}{2V_1^2+V_2^2}\left(\frac{a}{R_1}+\frac{a}{R_2}\right)\int d^2\vec{\mathbf{r}}\left(-\Psi^\dagger_{AK'\downarrow}(\vec{\mathbf{r}})\Psi_{BK'\uparrow}(\vec{\mathbf{r}})+\Psi^\dagger_{BK'\uparrow}\Psi_{AK'\downarrow}\right)$$

$$\mathcal{H}_{\mathcal{E}K\pi} \equiv -i\frac{2\sqrt{2}}{3}\frac{\Delta\lambda e\mathcal{E}V_2}{2V_1^2+V_2^2}\int d^2\vec{\mathbf{r}}\left(\Psi^\dagger_{AK\uparrow}(\vec{\mathbf{r}})\Psi_{BK\downarrow}(\vec{\mathbf{r}})-\Psi^\dagger_{BK\downarrow}\Psi_{AK\uparrow}\right).$$

$$\mathcal{H}_{\mathcal{E}K'\pi} \equiv -i\frac{2\sqrt{2}}{3}\frac{\Delta\lambda e\mathcal{E}V_2}{2V_1^2+V_2^2}\int d^2(\vec{\mathbf{r}})\left(-\Psi^\dagger_{AK'\downarrow}(\vec{\mathbf{r}})\Psi_{BK'\uparrow}(\vec{\mathbf{r}})+\Psi^\dagger_{BK'\uparrow}\Psi_{AK'\downarrow}\right).$$

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Effective Hamiltonian

Order Δ

$$\mathcal{H}_{\mathrm{RK}\pi} = -i\Delta_R \int d^2\vec{\mathbf{r}}\Psi_K^\dagger[\hat{\sigma}_+\hat{s}_+ - \hat{\sigma}_-\hat{s}_-]\Psi_K = \frac{\Delta_{\mathrm{R}}}{2}\int d^2\vec{\mathbf{r}}\Psi_K^\dagger[\hat{\sigma}_x\hat{s}_y + \hat{\sigma}_y\hat{s}_x]\Psi_K$$

$$\mathcal{H}_{\mathrm{RK}'\pi} = -i\Delta_R \int d^2\vec{\mathbf{r}}\Psi_{K'}^\dagger[-\hat{\sigma}_+\hat{s}_- + \hat{\sigma}_-\hat{s}_+]\Psi_{K'} = \frac{\Delta_{\mathrm{R}}}{2}\int d^2\vec{\mathbf{r}}\Psi_{K'}^\dagger[\hat{\sigma}_x\hat{s}_y - \hat{\sigma}_y\hat{s}_x]\Psi_{K'}$$

$$\Psi_{K(K')} = \begin{pmatrix} \Psi_{A\uparrow}(\vec{\mathbf{r}}) \\ \Psi_{A\downarrow}(\vec{\mathbf{r}}) \\ \Psi_{B\uparrow}(\vec{\mathbf{r}}) \\ \Psi_{B\downarrow}(\vec{\mathbf{r}}) \end{pmatrix}_{K(K')}$$

$$\begin{aligned} \Delta_R &= \Delta_{\mathcal{E}} + \Delta_{\mathrm{curv}} \\ \Delta_{\mathcal{E}} &= \frac{\Delta V_2}{2V_1^2 + V_2^2}\left[\frac{2\sqrt{2}}{3}\lambda e\mathcal{E}\right] \simeq \frac{2\sqrt{2}}{3}\frac{\Delta\lambda e\mathcal{E}}{V_2} \\ \Delta_{\mathrm{curv}} &= \frac{\Delta V_1}{2V_1^2 + V_2^2}\left[(V_{pp\sigma} - V_{pp\pi})\left(\frac{a}{R_1} + \frac{a}{R_2}\right)\right] \simeq \frac{\Delta(V_{pp\sigma} - V_{pp\pi})}{V_1}\left(\frac{a}{R_1} + \frac{a}{R_2}\right)\left(\frac{V_1}{V_2}\right)^2 \end{aligned}$$

$V_1 \ll V_2$ (widely separated σ bands)

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Effective Hamiltonian

Order Δ^2

$$\mathcal{H}_{\mathrm{int}K(K')} = \pm\ \Delta_{\mathrm{int}} \times$$

$$\int d^2\vec{\mathbf{r}}\Psi^{\dagger}_{AK(K')\uparrow}(\vec{\mathbf{r}})\Psi_{AK(K')\uparrow}(\vec{\mathbf{r}}) - \Psi^{\dagger}_{AK(K')\downarrow}(\tilde{\mathbf{r}})\Psi_{AK(K')\downarrow}(\vec{\mathbf{r}})$$

$$- \Psi^{\dagger}_{BK(K')\uparrow}(\vec{\mathbf{r}})\Psi_{BK(K')\uparrow}(\vec{\mathbf{r}}) + \Psi_{BK(K')\downarrow}(\vec{\mathbf{r}})\Psi_{BK(K')\downarrow}(\vec{\mathbf{r}})$$

$$\Delta_{\mathrm{int}} = \frac{3}{4}\frac{\Delta^2}{V_1}\frac{V_1^4}{(V_2^2 - V_1^2)(2V_1^2 + V_2^2)} \simeq \frac{3}{4}\frac{\Delta^2}{V_1}\left(\frac{V_1}{V_2}\right)^4$$

$V_1 \ll V_2$ (widely separated σ bands)

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Effective Hamiltonian for graphene

$$\mathcal{H}_T = \int d^2\vec{\mathbf{r}}\Psi^\dagger \left(-i\hbar v_F[\hat{\sigma}_y\hat{\partial}_x - \hat{\tau}_z\hat{\sigma}_x\hat{\partial}_y] + \Delta_{\text{int}}[\hat{\tau}_z\hat{\sigma}_z\hat{s}_z] + \frac{\Delta_R}{2}[\hat{\sigma}_x\hat{s}_y + \hat{\tau}_z\hat{\sigma}_y\hat{s}_x]\right)\Psi$$

- We obtain an effective Hamiltonian equivalent to the one of Kane &Mele PRL **95**,226801 (2005).
- Y. Yao *et al.*, cond-mat/0606350 : Δ_{int}
- H. Min *et al.*, cond-mat/0606504 : $\Delta_R = \Delta_\varepsilon$ but no Δ_{curv}

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Estimates

$\hbar v_F = \sqrt{3}\gamma_o a/2$	a ~ 2.46 Å	$\gamma_o \sim 3$eV	$V_{pp\pi} \sim -2.24$eV
$\mathcal{E} \approx 50$V/300nm	$\lambda = 3a_o/Z \approx 0.264$Å	$\Delta = 12$meV	
$V_{sp\sigma} \sim 4.2$eV	$V_{ss\sigma} \sim -3.63$eV	$V_{pp\sigma} \sim 5.38$eV	
$V_1 = 2.47$eV $V_2 = 6.33$eV	$a = 1.42$Å $l \sim 100$ Å $h \sim 10$ Å $R \sim 50 - 100$nm		

$\frac{3}{4}\frac{\Delta^2}{V_1}\left(\frac{V_1}{V_2}\right)^4$	0.01K
$\frac{2\sqrt{2}}{3}\frac{\Delta\lambda e\mathcal{E}}{V_2}$	0.07K
$\frac{\Delta(V_{pp\sigma}-V_{pp\pi})}{V_1}\left(\frac{a}{R_1}+\frac{a}{R_2}\right)\left(\frac{V_1}{V_2}\right)^2$	0.2K

Kane & Mele

$\Delta_{\text{int}} \sim 2.4K$

$\Delta_\varepsilon \sim 2.5mK$

(!!?)

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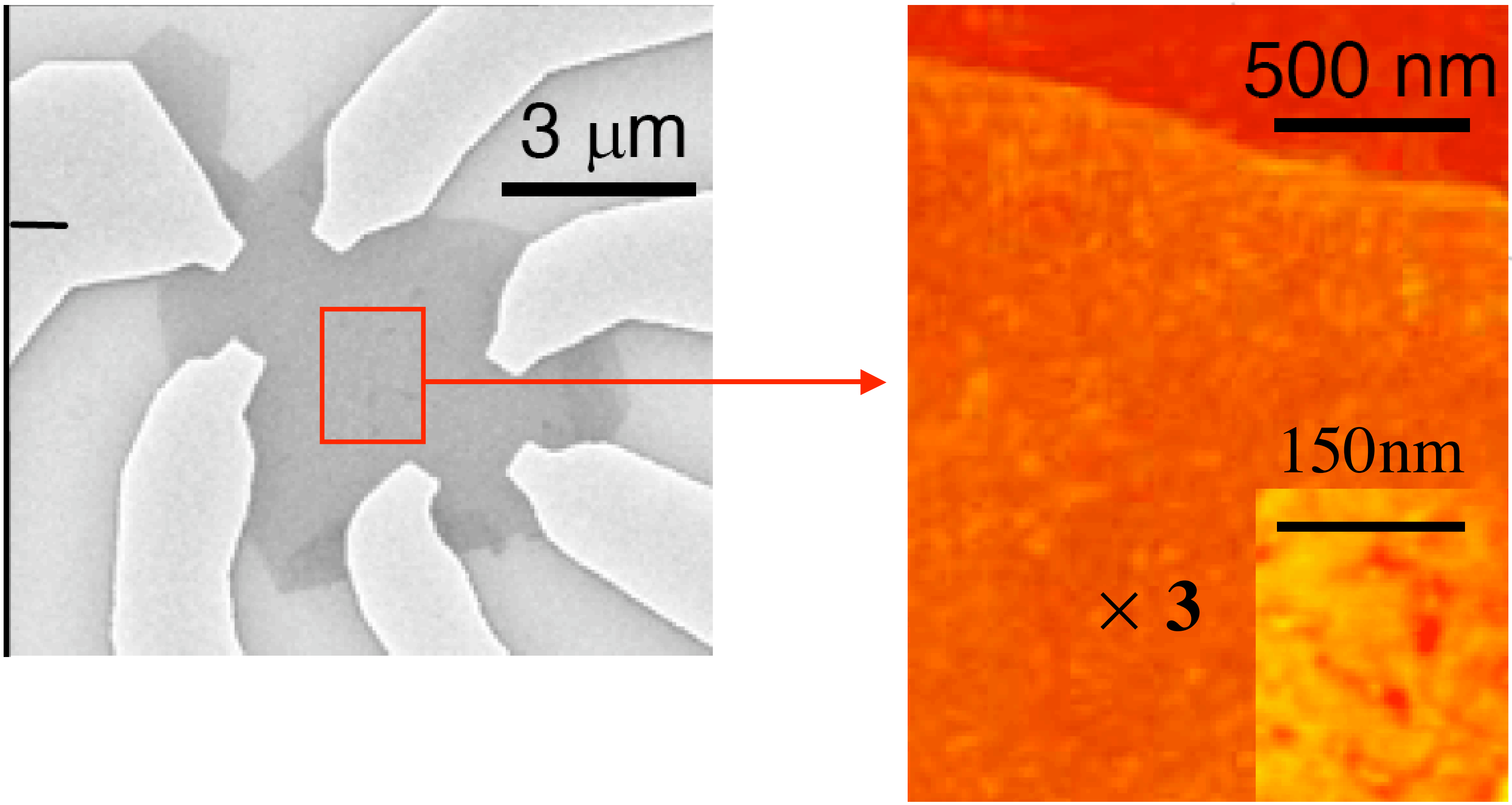
Estimates for ripples curvature

ripples of lateral size ranging 50nm -100nm



K. Novoselov *et. al.*, Science **306**, 666 (2004);
Nature **438**,197 (2005);
S.V. Morozov *et. al.*, PRL **97**, 016801 (2006)

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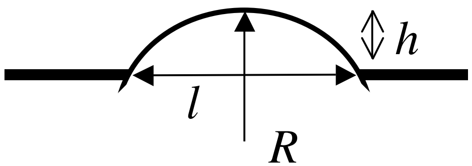
Estimates for ripples curvature

ripples of lateral size ranging 50nm -100nm

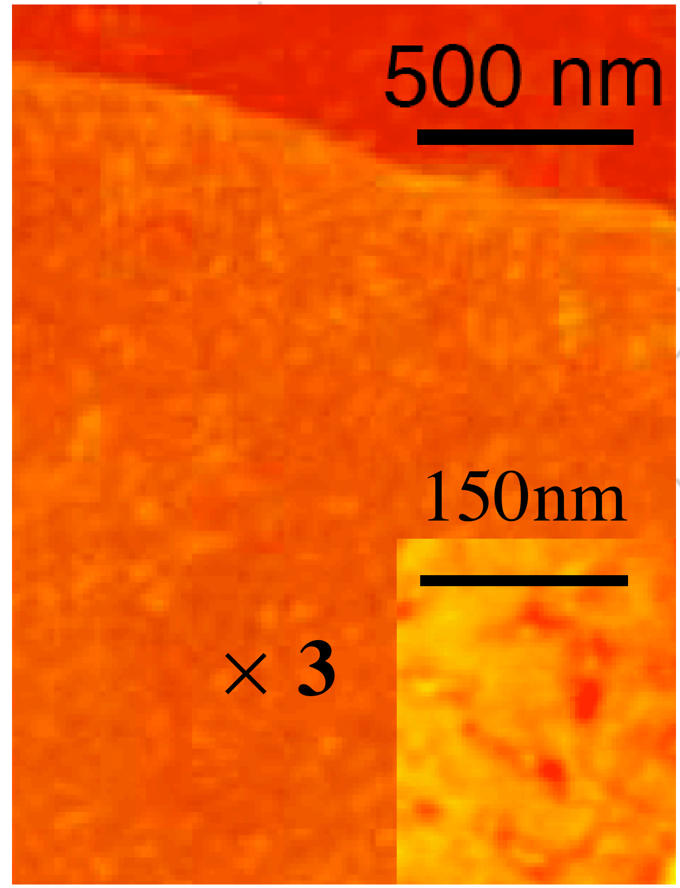
1)



$h \ll R$

$l \approx R$

$R_1 \sim R_2 \sim 50 - 100\text{nm}$



2)

A. F. Morpurgo and F. Guinea,
cond-mat/0603789
Random elastic strain

$R^{-1} \sim h/l^2 \quad l \sim 100\ \text{Å}$

$h \sim 10\ \text{Å}$

$R_1 \sim R_2 \sim 100\text{nm}$

$\Delta_{\text{curv}} \sim 1.22 \times 10^{-5}\text{eV} \rightarrow 0.14\ \text{K}$

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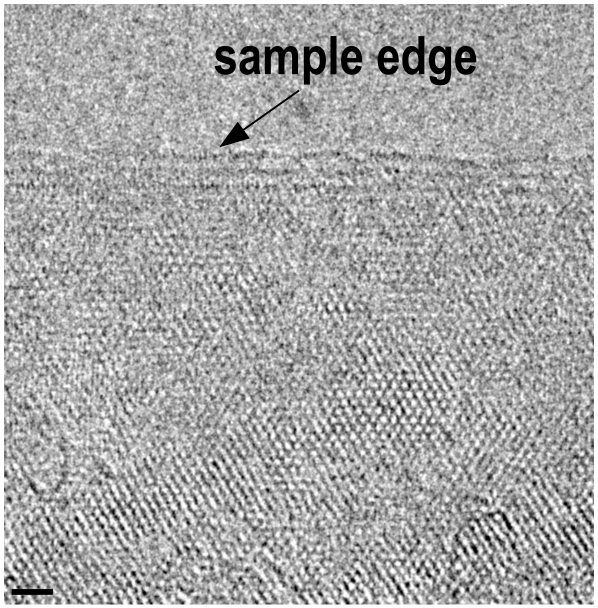
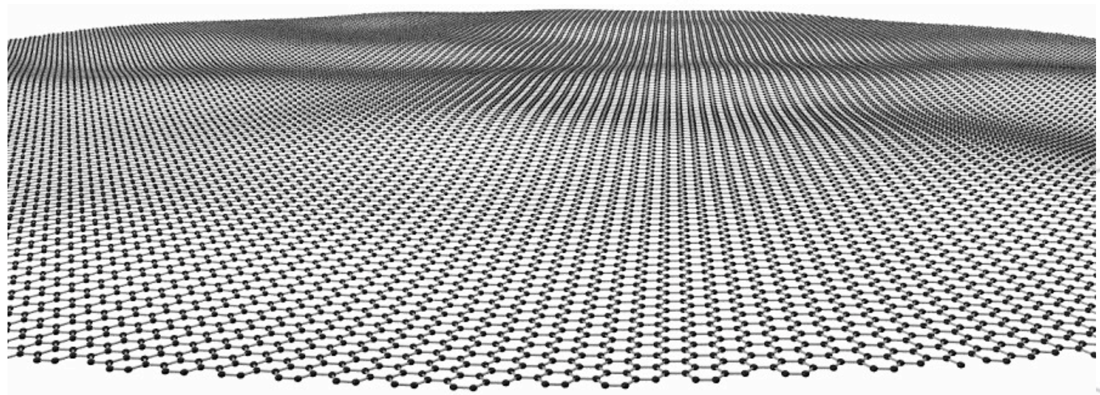
Intrinsic Microscopic Crumpling

atomic resolution TEM

ripple contrast appears for >1 layer



Courtesy of A. Geim&D. Obergfell



height ≈5Å; size <5nm;
strain ≈1%

Nelson (1987, 2004):

2D membranes can be stabilized by intrinsic crumpling in 3D

- buckling (dislocations would destroy mobility)
- bending (elastic strain)

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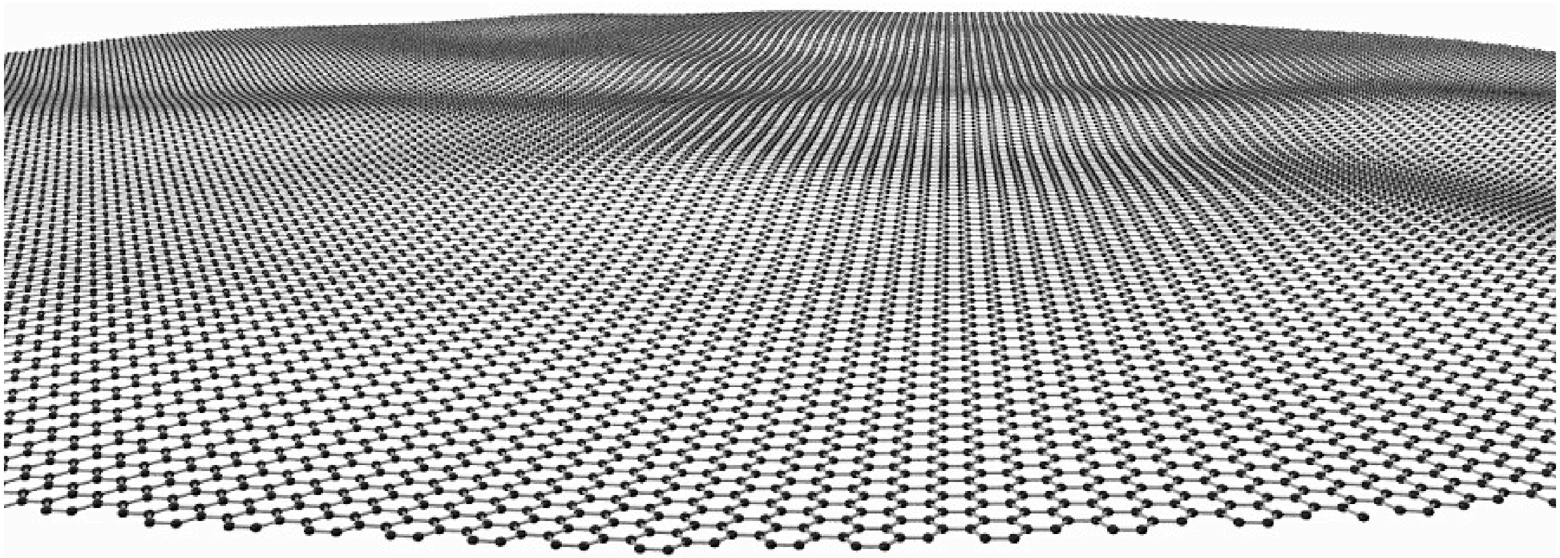
Estimates for ripples curvature



$$l \approx 5\text{nm} \qquad h \approx 0.5\text{nm} \qquad R \approx \frac{l^2}{h} = 50\text{nm}$$

$$\Delta_{\text{curv}} \sim 0.28\text{K}$$

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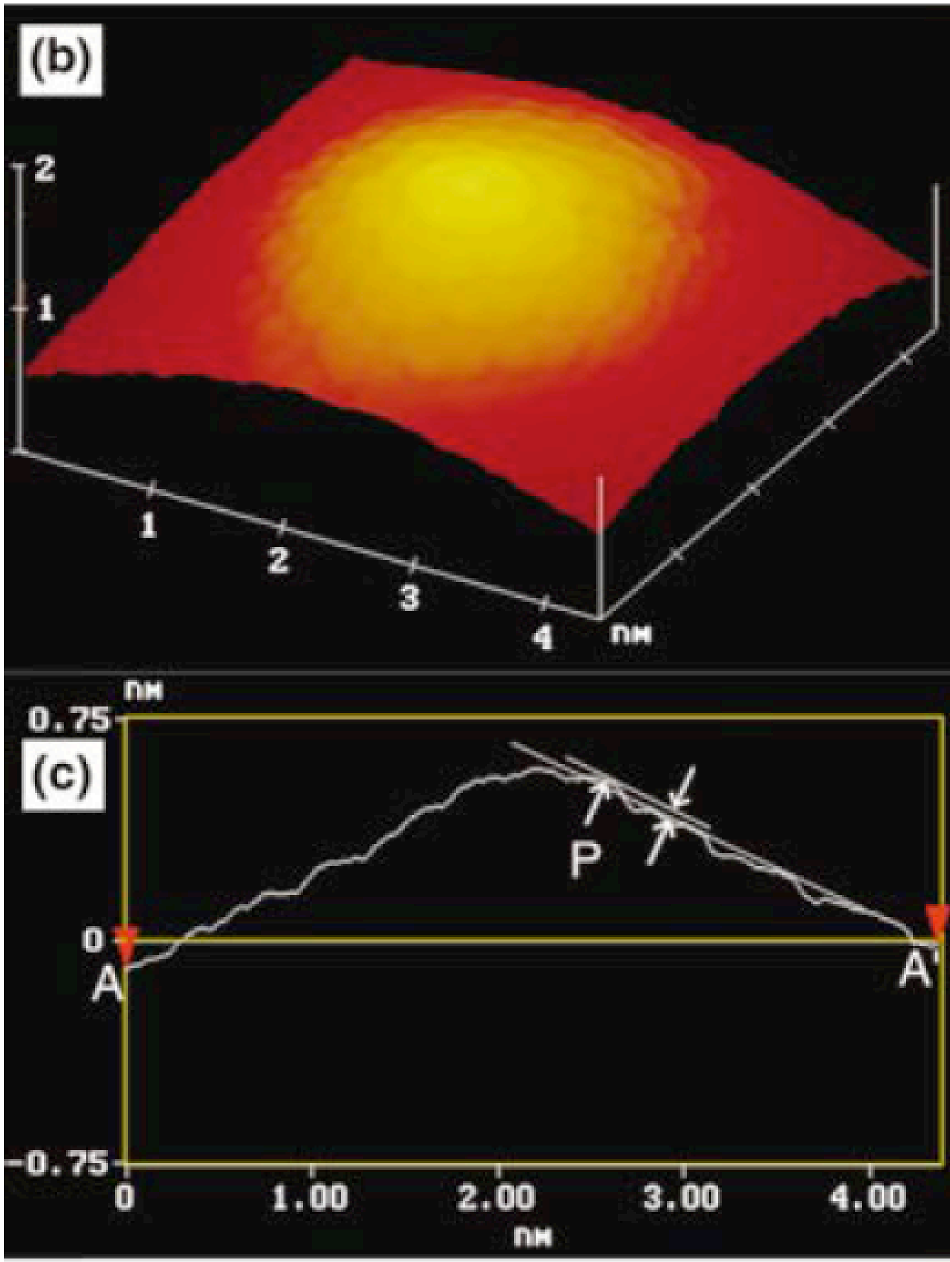
Estimates for ripples curvature



B. An *et. al.*,
Appl. Phys. Lett. **78**, 3696, (2001)

$l \approx 5\text{nm} \qquad h \approx 0.5\text{nm}$

$$R \approx \frac{l^2}{h} = 50\text{nm}$$

$$\Delta_{\text{curv}} \sim 0.28\text{K}$$

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Fullerenes

$$|+1\,s\,\mathcal{K}\rangle \equiv \sqrt{\frac{3}{4\pi}}\cos^2\left(\frac{\theta}{2}\right)e^{i\phi}\begin{pmatrix}|AK\rangle\\ i|BK'\rangle\end{pmatrix}\otimes|s\rangle$$

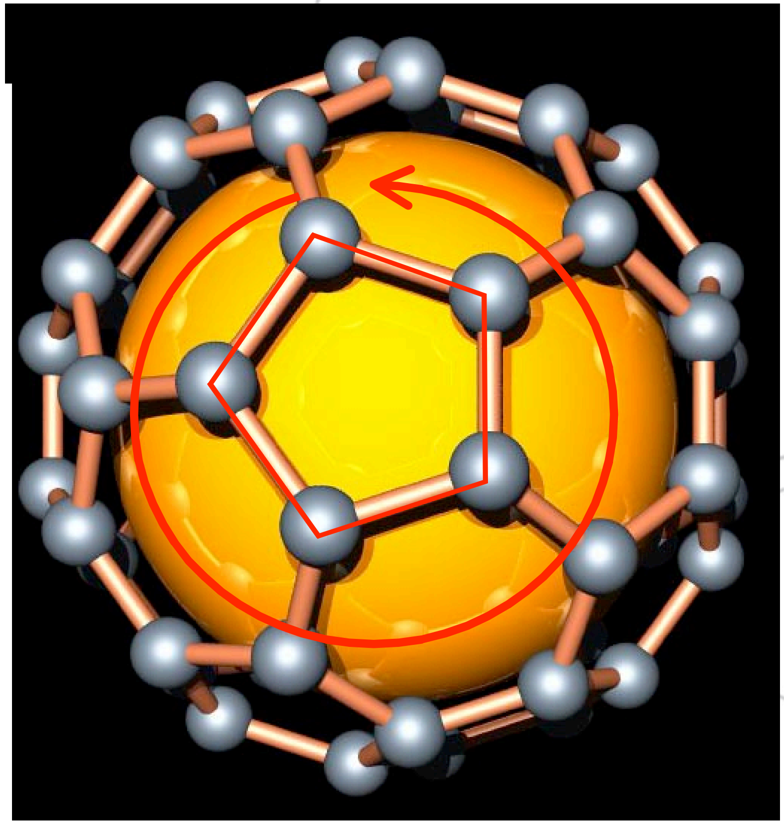
$$|0\,s\,\mathcal{K}\rangle \equiv \sqrt{\frac{3}{2\pi}}\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)\begin{pmatrix}|AK\rangle\\ i|BK'\rangle\end{pmatrix}\otimes|s\rangle$$

$$|-1\,s\,\mathcal{K}\rangle \equiv \sqrt{\frac{3}{4\pi}}\sin^2\left(\frac{\theta}{2}\right)e^{-i\phi}\begin{pmatrix}|AK\rangle\\ i|BK'\rangle\end{pmatrix}\otimes|s\rangle$$

$$|+1\,s\,\mathcal{K}'\rangle \equiv \sqrt{\frac{3}{4\pi}}\sin^2\left(\frac{\theta}{2}\right)e^{i\phi}\begin{pmatrix}|AK\rangle\\ -i|BK'\rangle\end{pmatrix}\otimes|s\rangle$$

$$|0\,s\,\mathcal{K}'\rangle \equiv -\sqrt{\frac{3}{2\pi}}\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)\begin{pmatrix}|AK\rangle\\ -i|BK'\rangle\end{pmatrix}\otimes|s\rangle$$

$$|-1\,s\,\mathcal{K}'\rangle \equiv \sqrt{\frac{3}{4\pi}}\cos^2\left(\frac{\theta}{2}\right)e^{-i\phi}\begin{pmatrix}|AK\rangle\\ -i|BK'\rangle\end{pmatrix}\otimes|s\rangle$$



$$\tilde{\Psi}_{A\mathcal{K}\tilde{\mathbf{k}}s}(\tilde{\mathbf{r}}) = \Psi_{AK\tilde{\mathbf{k}}s}(\tilde{\mathbf{r}}) + i\Psi_{BK'\tilde{\mathbf{k}}s}(\tilde{\mathbf{r}})$$

$$\tilde{\Psi}_{B\mathcal{K}'\tilde{\mathbf{k}}s}(\tilde{\mathbf{r}}) = -i\ \Psi_{BK'\tilde{\mathbf{k}}s}(\tilde{\mathbf{r}}) + \Psi_{AK\tilde{\mathbf{k}}s}(\tilde{\mathbf{r}}).$$

González,Vozmediano,Guinea,
PRL **69**, 172 (1992)

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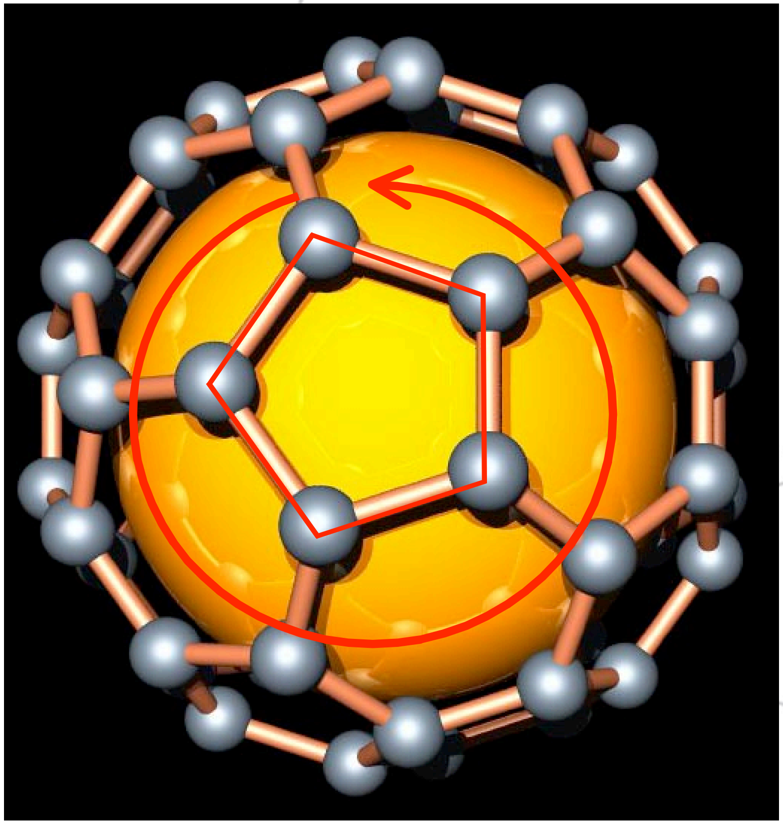
Fullerenes

$$|+1\uparrow\rangle, |+1\downarrow\rangle, |0\uparrow\rangle, |0\downarrow\rangle, |-1\uparrow\rangle, |-1\downarrow\rangle$$



$$\mathcal{H}^{\mathcal{K}}_{\mathrm{S-O\,int}} = \begin{pmatrix} \Delta_{\mathrm{int}} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\Delta_{\mathrm{int}} & \sqrt{2}\Delta_{\mathrm{int}} & 0 & 0 & 0 \\ 0 & \sqrt{2}\Delta_{\mathrm{int}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{2}\Delta_{\mathrm{int}} & 0 \\ 0 & 0 & 0 & \sqrt{2}\Delta_{\mathrm{int}} & -\Delta_{\mathrm{int}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \Delta_{\mathrm{int}} \end{pmatrix}$$

$$\epsilon = +\Delta_{\mathrm{int}} \rightarrow \Psi_{\Delta} : \{|+1\uparrow\rangle, |-1\downarrow\rangle, \sqrt{\frac{1}{3}}|+1\downarrow\rangle + \sqrt{\frac{2}{3}}|0\uparrow\rangle, \sqrt{\frac{1}{3}}|-1\uparrow\rangle + \sqrt{\frac{2}{3}}|0\downarrow\rangle\}$$

$$\epsilon = -2\Delta_{\mathrm{int}} \rightarrow \Psi_{-2\Delta} : \{\sqrt{\frac{2}{3}}|+1\downarrow\rangle - \sqrt{\frac{1}{3}}|0\uparrow\rangle, \sqrt{\frac{2}{3}}|-1\uparrow\rangle - \sqrt{\frac{1}{3}}|0\downarrow\rangle\}$$

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Nanotubes

H=

$$\begin{pmatrix} 0 & \hbar v_{\mathrm{F}}(k - in/R) + \tau\ i\Delta_R \pi \hat{s}_z \\ \hbar v_{\mathrm{F}}(k + in/R) - \tau\ i\Delta_R \pi \hat{s}_z & 0 \end{pmatrix}$$

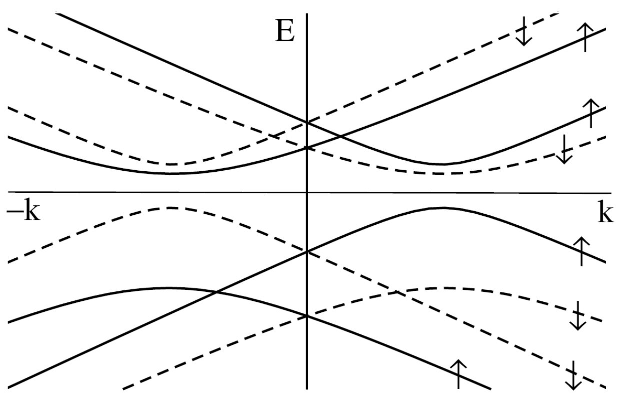
T. Ando, JPSJ **69**, 1757 (2000).

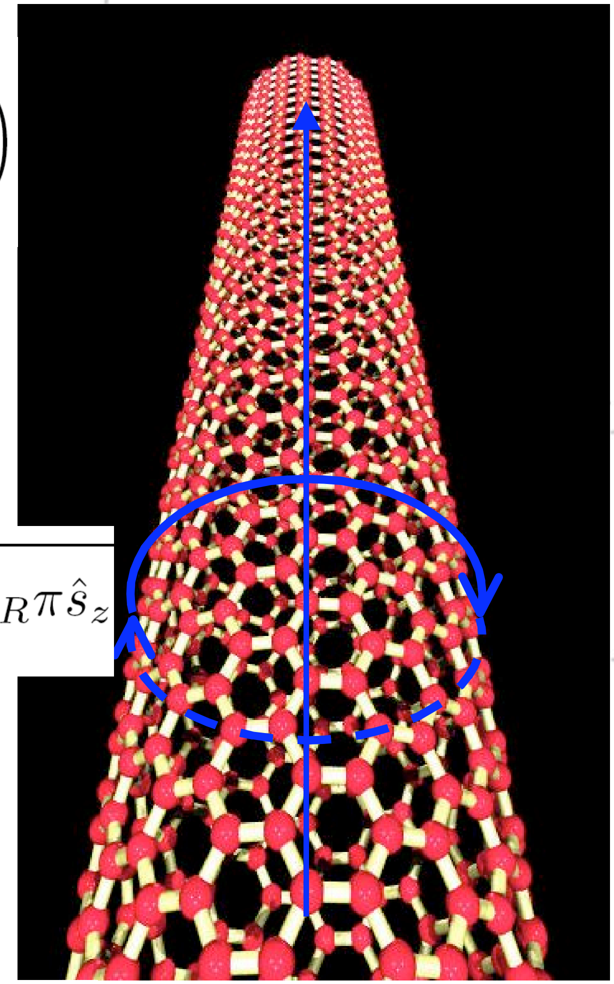
A. De Martino *et. al.*,PRL **88**, 206402 (2002)

$$\epsilon_k = \pm\sqrt{(\pi\Delta_{\mathrm{R}})^2 + (v_{\mathrm{F}} k)^2}. \quad n = 0 \text{ Gap}$$

$$\epsilon_k = \pm\sqrt{(\pi\Delta_{\mathrm{R}})^2 + (\hbar v_{\mathrm{F}})^2 (k^2 + (n/R)^2) + 2(n/R)\hbar v_{\mathrm{F}} \Delta_R \pi \hat{s}_z}$$

$n \neq 0$ Spin-splitting





$R_1 \sim 6, 12, 24\text{Å} \quad \Delta_R \sim 12, 6, 3\text{K}$

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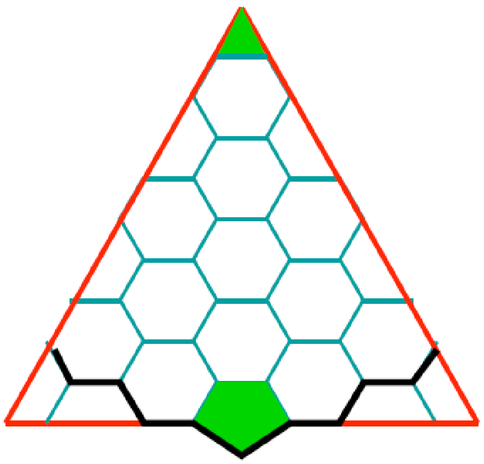
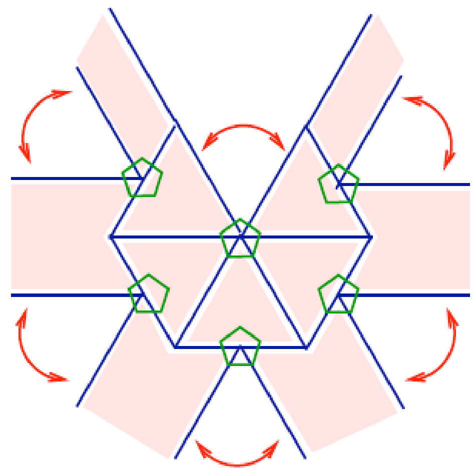
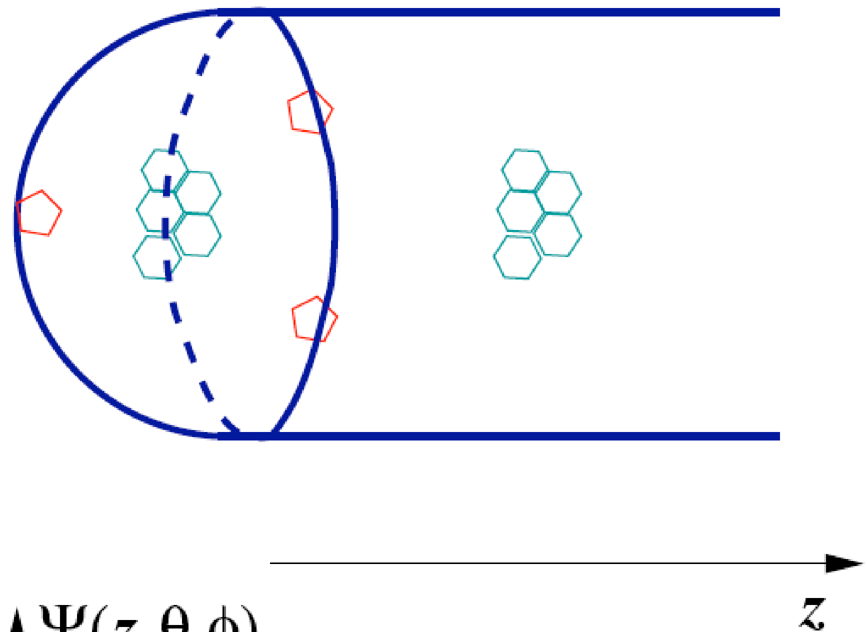
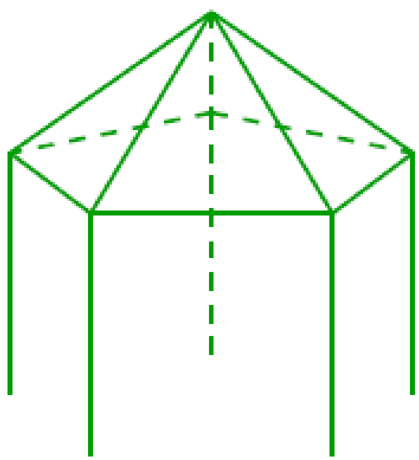
L. Chico *et. al.*,PRL **93**, 176402 (2004)

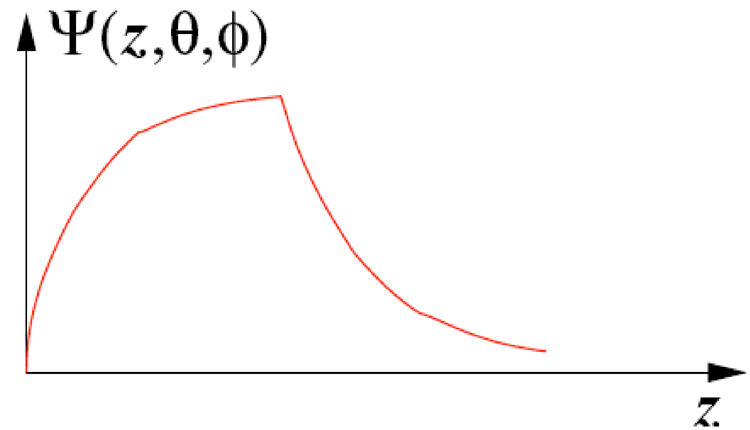
Fullerenes+Nanotubes: Cap states











Fullerenes+Nanotubes: Cap states

$$|+1\,s\rangle_A \equiv \frac{1}{\sqrt{2}}(|+1\,s\,\mathcal{K}\rangle + |+1\,s\,\mathcal{K}'\rangle) = \sqrt{\frac{3}{8\pi}}e^{i\phi}\begin{pmatrix}|AK\rangle\\ 0\end{pmatrix}\otimes|s\rangle$$

$$|-1\,s\rangle_A \equiv \frac{1}{\sqrt{2}}(|-1\,s\,\mathcal{K}\rangle + |-1\,s\,\mathcal{K}'\rangle) = \sqrt{\frac{3}{8\pi}}e^{-i\phi}\begin{pmatrix}|AK\rangle\\ 0\end{pmatrix}\otimes|s\rangle$$

$$|+1\,s\rangle_B \equiv \frac{1}{\sqrt{2}}(|+1\,s\,\mathcal{K}\rangle - |+1\,s\,\mathcal{K}'\rangle) = \sqrt{\frac{3}{8\pi}}e^{i\phi}\begin{pmatrix}0\\ i|BK'\rangle\end{pmatrix}\otimes|s\rangle$$

$$|-1\,s\rangle_B \equiv \frac{1}{\sqrt{2}}(|-1\,s\,\mathcal{K}\rangle - |-1\,s\,\mathcal{K}'\rangle) = \sqrt{\frac{3}{8\pi}}e^{-i\phi}\begin{pmatrix}0\\ i|BK'\rangle\end{pmatrix}\otimes|s\rangle$$

$$|+1, s = \uparrow,\downarrow\rangle_B \rightarrow \epsilon_{\uparrow,\downarrow} = \pm\Delta_{\mathrm{int}}$$

$$|-1, s = \uparrow,\downarrow\rangle_B \rightarrow \epsilon_{\uparrow,\downarrow} = \mp\Delta_{\mathrm{int}}.$$

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Fullerenes+Nanotubes: Cap states

$$\Psi_{m=2}(z,\phi) \equiv \frac{C}{4\sqrt{2\pi}} e^{2i\phi} e^{\kappa z/R} \begin{pmatrix} |K\rangle - |K'\rangle \\ i|K\rangle + i|K'\rangle \end{pmatrix}$$

$$C^{-2} = \frac{13}{16} + \frac{1}{4\kappa} \qquad \kappa^2 = n^2 - \frac{\epsilon^2 R^2}{v_{\mathrm{F}}^2}$$

$$\epsilon_{\mathrm{Rashba}} \approx \pm C^2 \Delta_{\mathrm{R}} \left(\frac{1}{16\kappa} + \frac{31}{80} \right) \approx \pm \frac{\Delta_{\mathrm{R}}}{4} \left(1 - \frac{59\kappa}{20} \right)$$

C_{60} fullerene of radius $R \sim 3.55$Å

$$\Delta_R/4 \sim 3\mathrm{K}$$

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Conclusions

- TB model+Atomic s-o→Effective s-o for π bands in graphene
- Atomic stark effect: Effective Rashba s-o ~ Δ
- Local Curvature: Extra "Rashba-like" s-o coupling ~ Δ
- Intrinsic ripples in Graphene:
  - Flat graphene +Pentagons. Topological defect.
- Intrinsic s-o coupling ~ Δ^2
- Our estimates: $\Delta_{curv} \sim 0.2K$, $\Delta_{\varepsilon} \sim 0.07K$, $\Delta_{\text{int}} \sim 10mK$ Kane&Mele different estimates!!
- Spin-orbit in Fullerenes, Nanotubes, Caps:
  - Curvature more pronounced
  - Topology also important

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