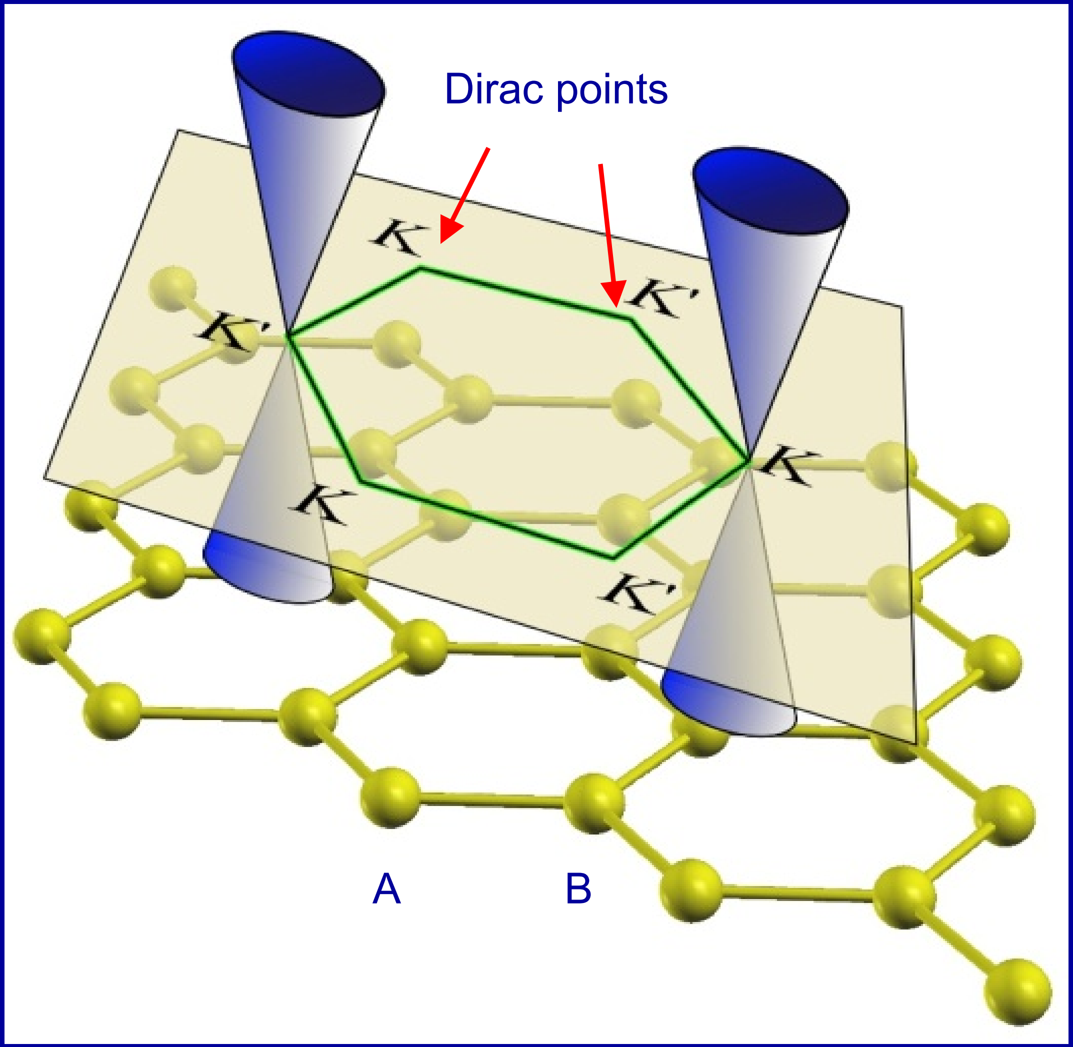
Spin-orbit coupling in graphene

Jaroslav Fabian

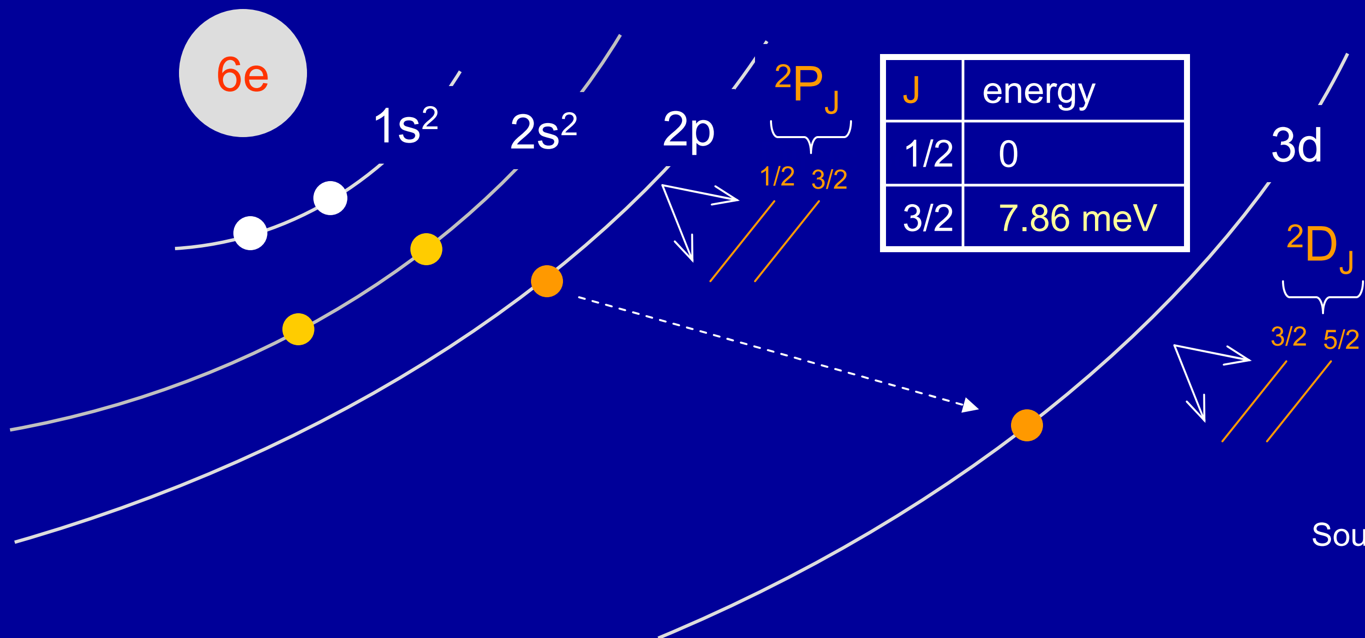
University of Regensburg

graphene 101



How conic are the cones?
How does spin-orbit coupling modifies the band structure topology?

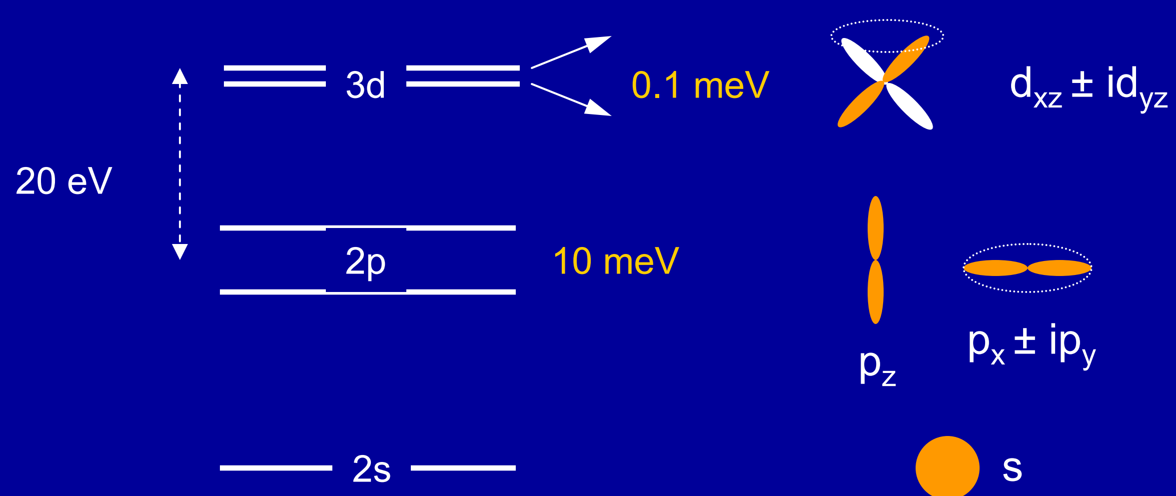
:spin-orbit splitting in the carbon ion $2s^2 2p$:



J	energy
1/2	0
3/2	7.86 meV

J	energy	diff.
3/2	18.0458 eV	0.2 meV
5/2	18.0460	

Source: NIST Atomic Spectra Database

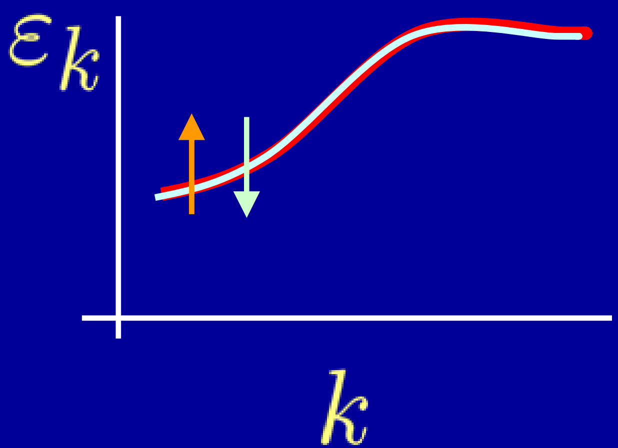


going to solids: intrinsic and extrinsic SOC

solids *with* space inversion symmetry

graphene, bilayer, ABC trilayer, graphite, …

silicon, aluminum, …



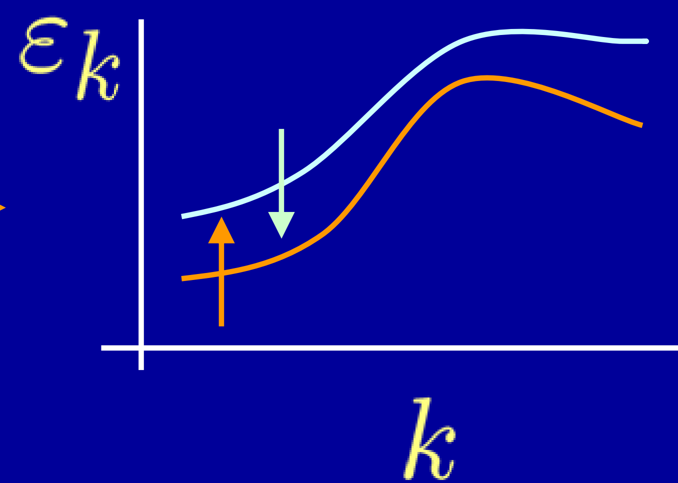
degeneracy at k

solids *without* space inversion symmetry

graphene in transverse electric field … *extrinsic*

graphene on a substrate … *extrinsic*

ABA trilayer … GaAs



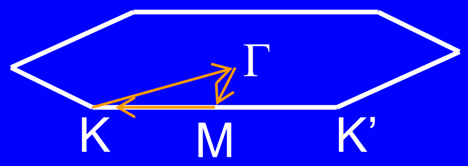
no degeneracy

(only Kramers left)

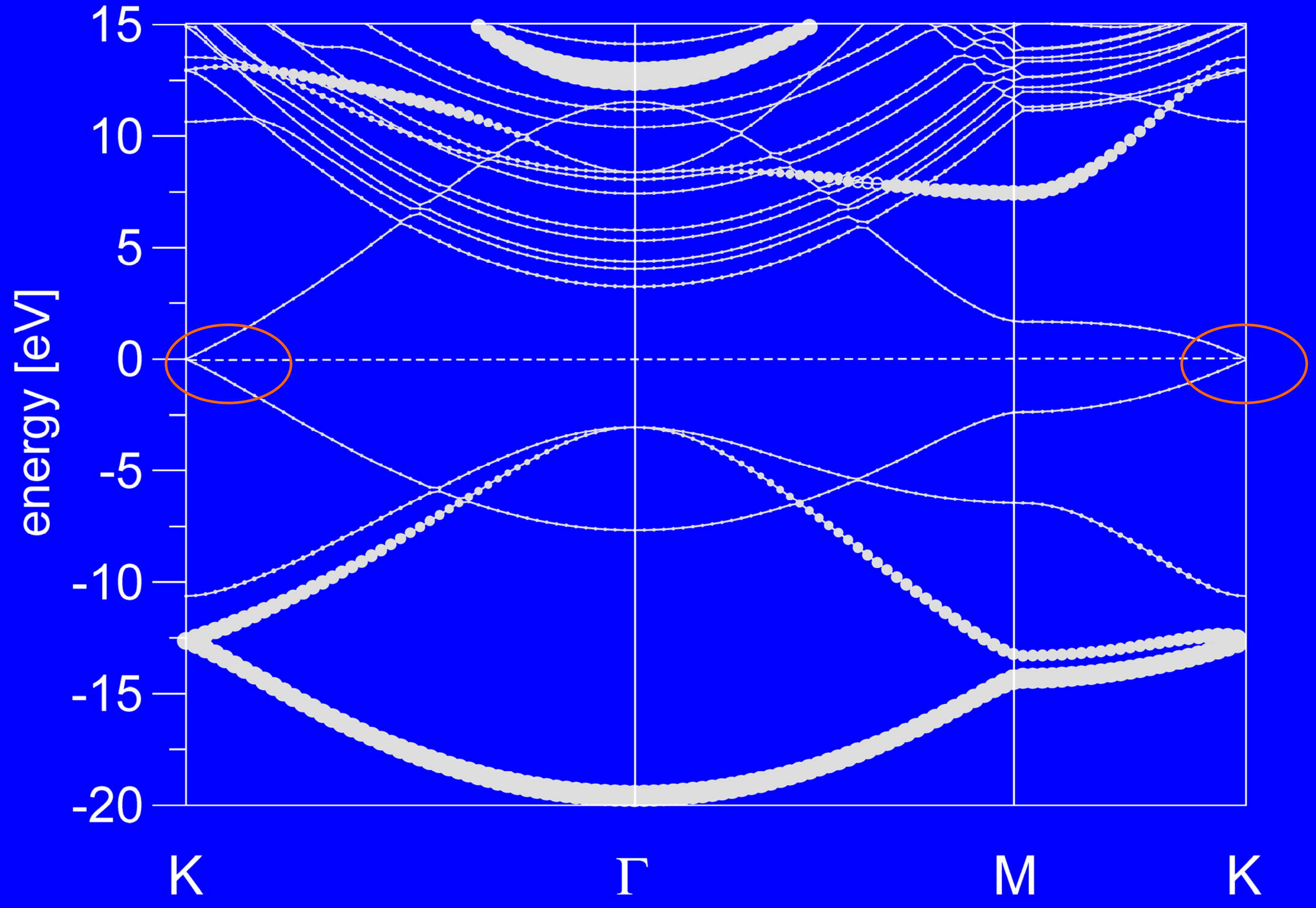
What are the functional forms (spectrum) of the spin-orbit field?

:graphene band structure:

character of the bands

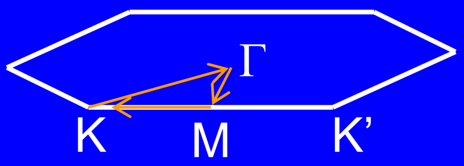


s character

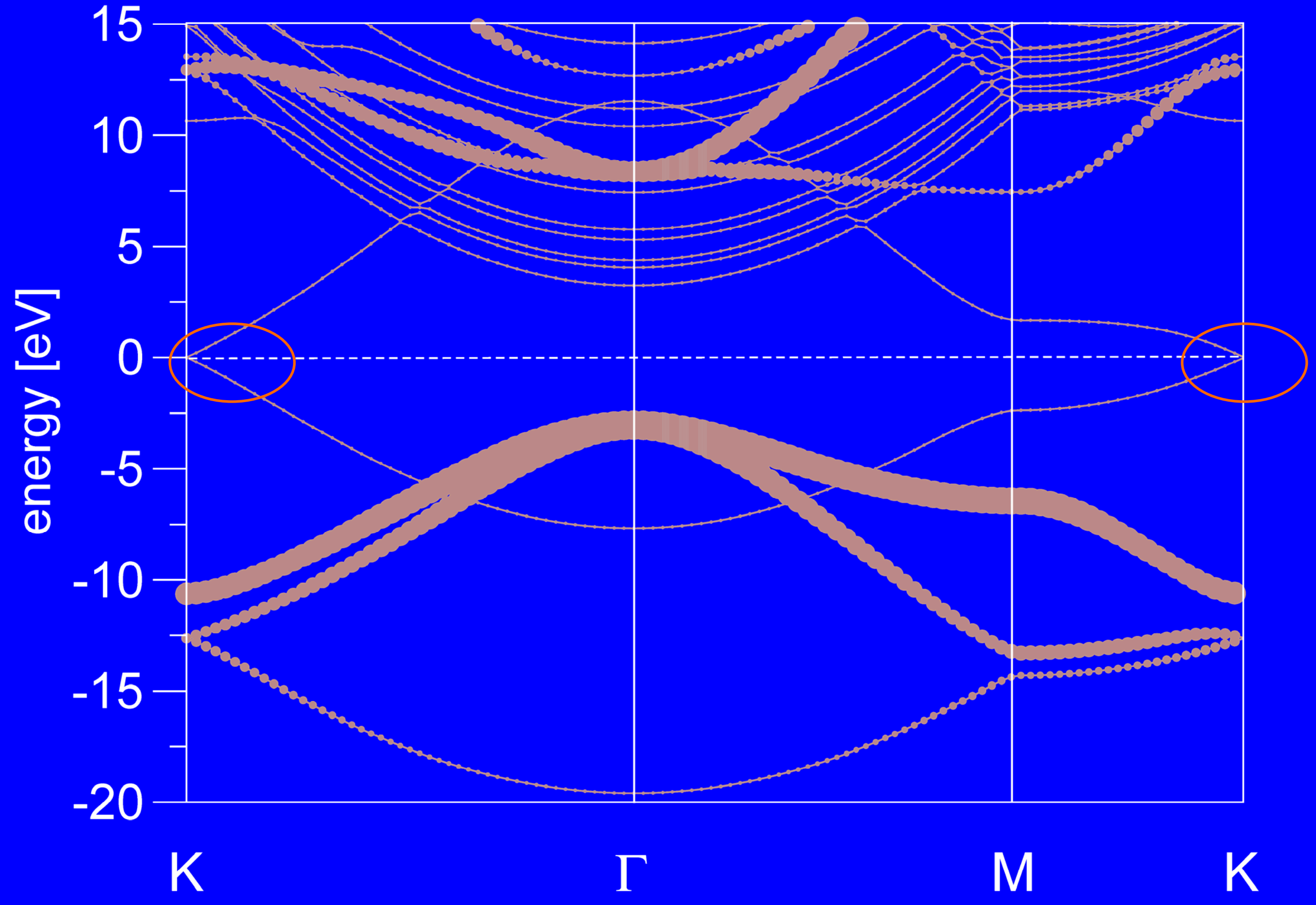


:graphene band structure:

character of the bands

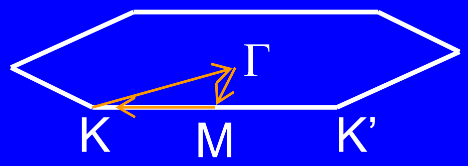


$p_{x,y}$ character

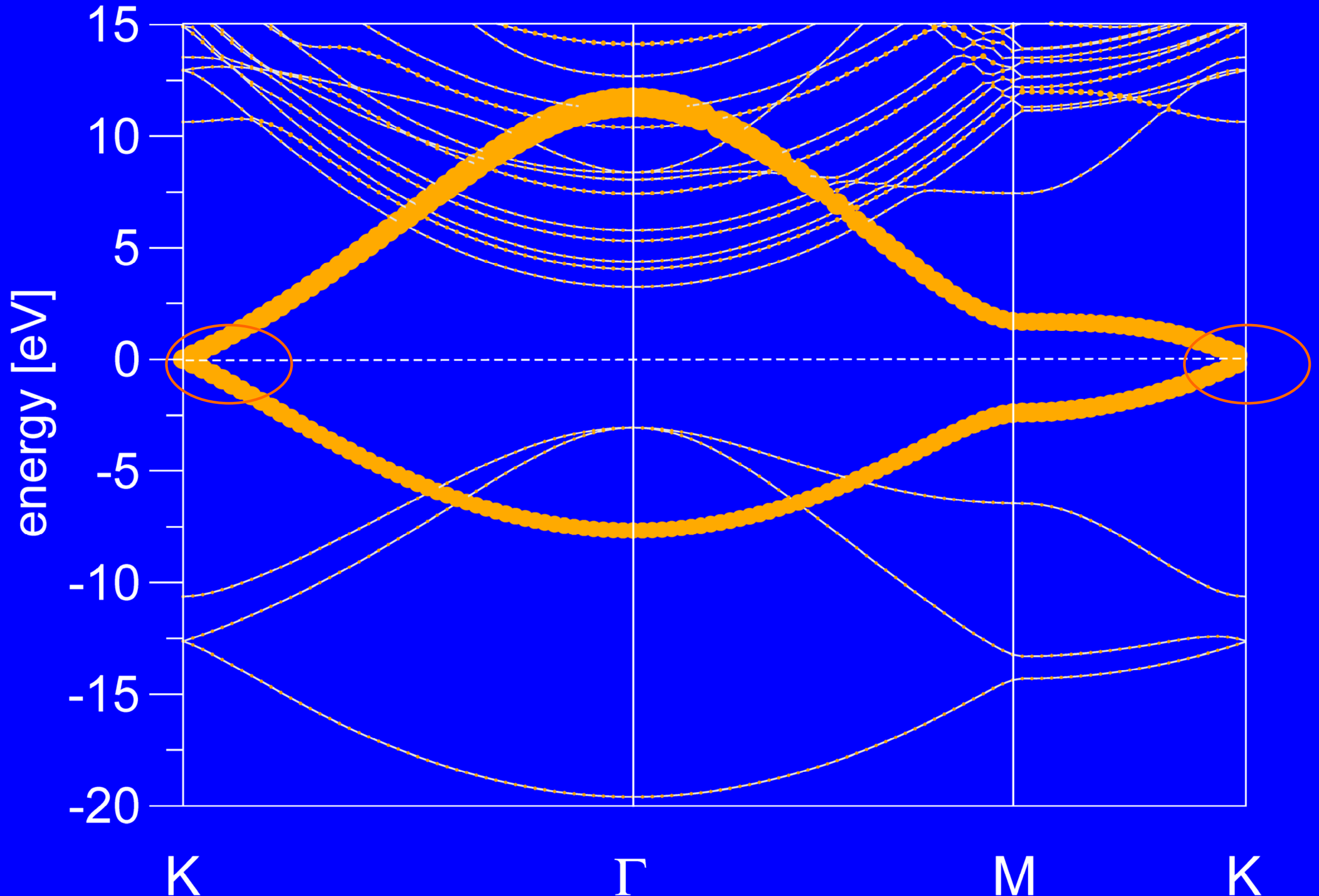


:graphene band structure:

character of the bands

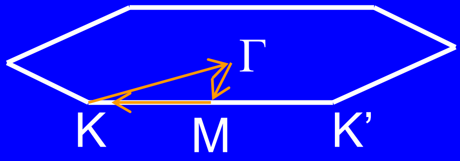


p_z character

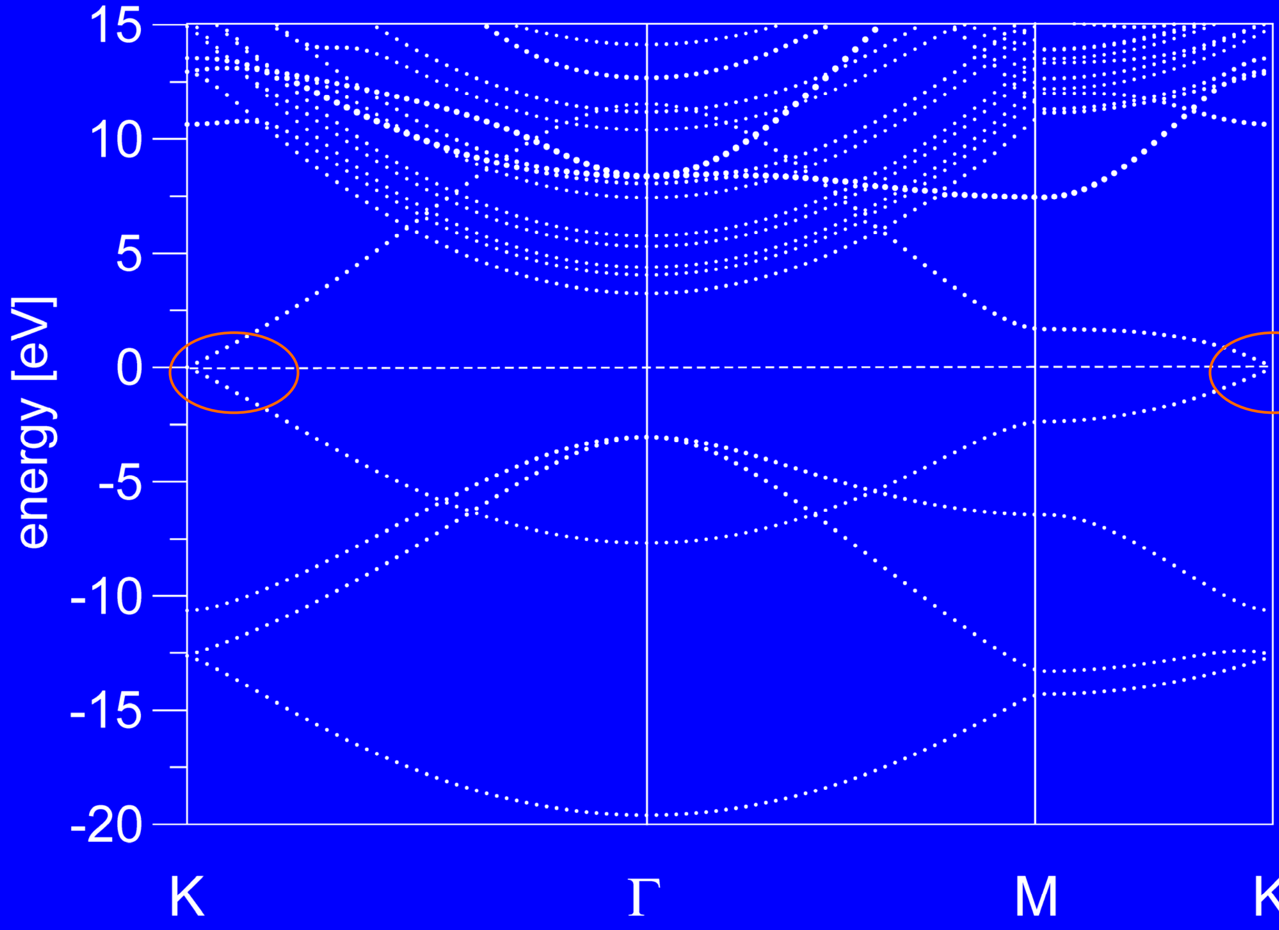


:graphene band structure:

character of the bands

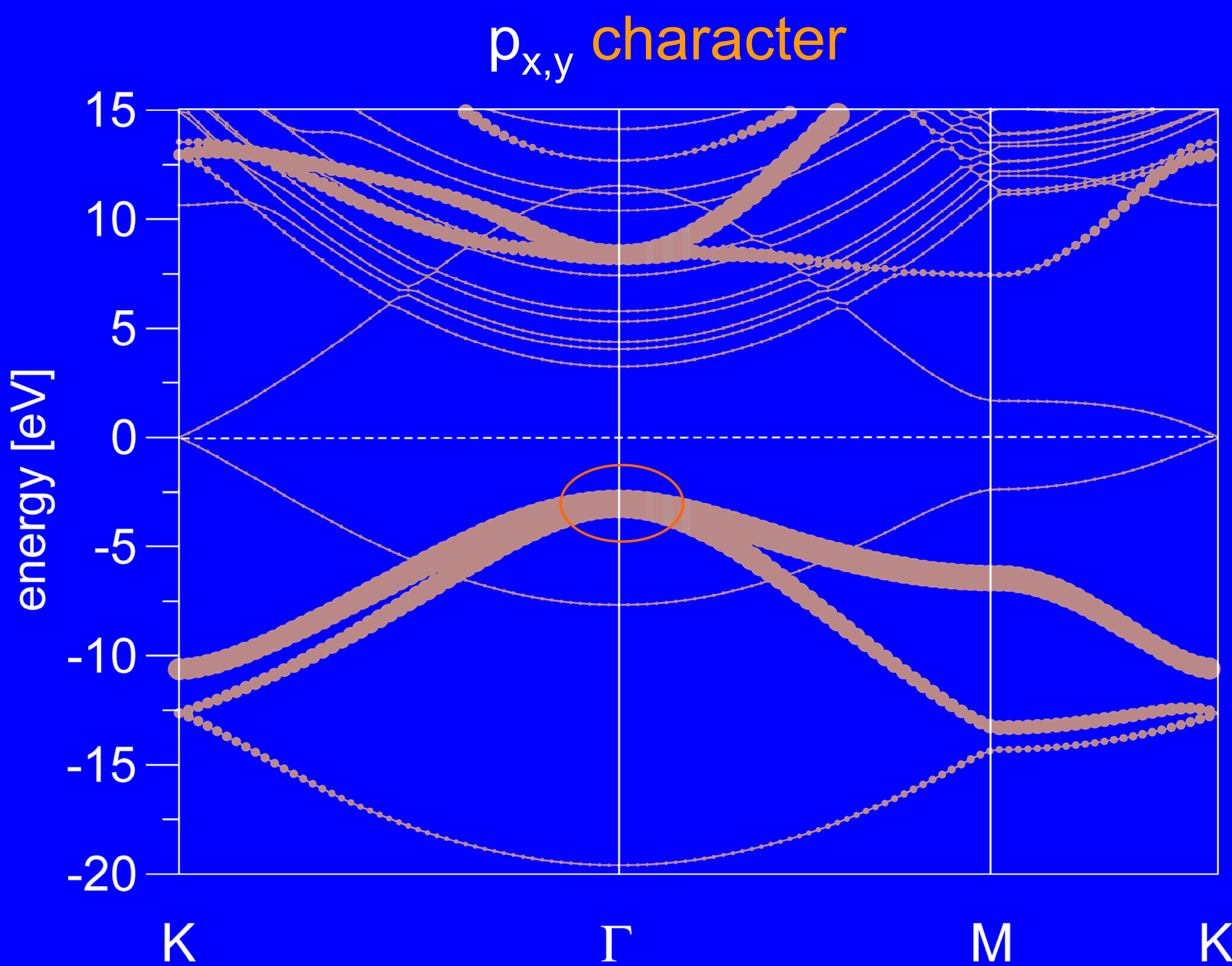


d character



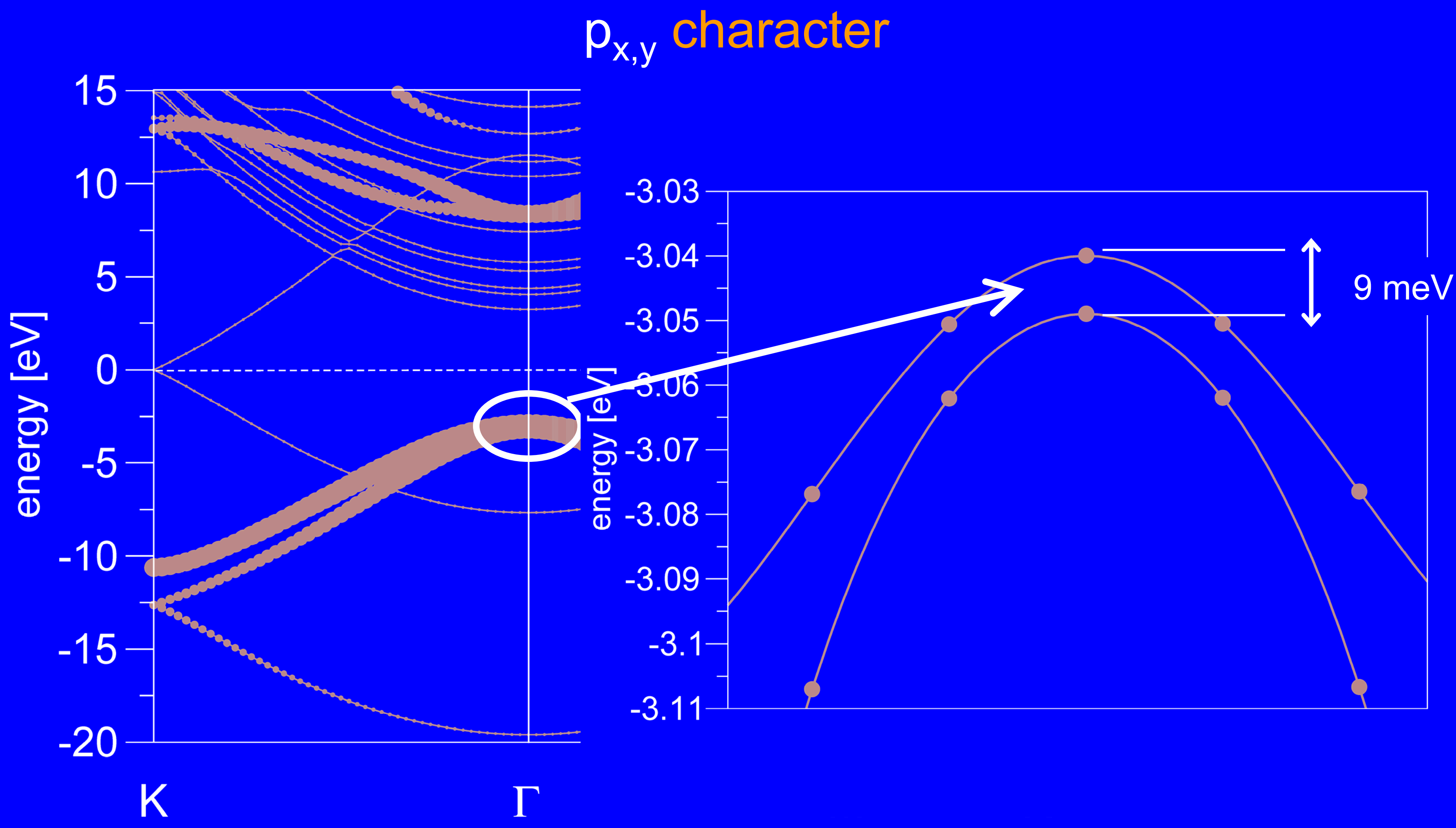
:graphene band structure:

Spin-orbit coupling at Γ: 9 meV



:graphene band structure:

spin-orbit coupling at Γ: ~ 10 meV, as in C atom



:spin-orbit coupling in graphene at K:

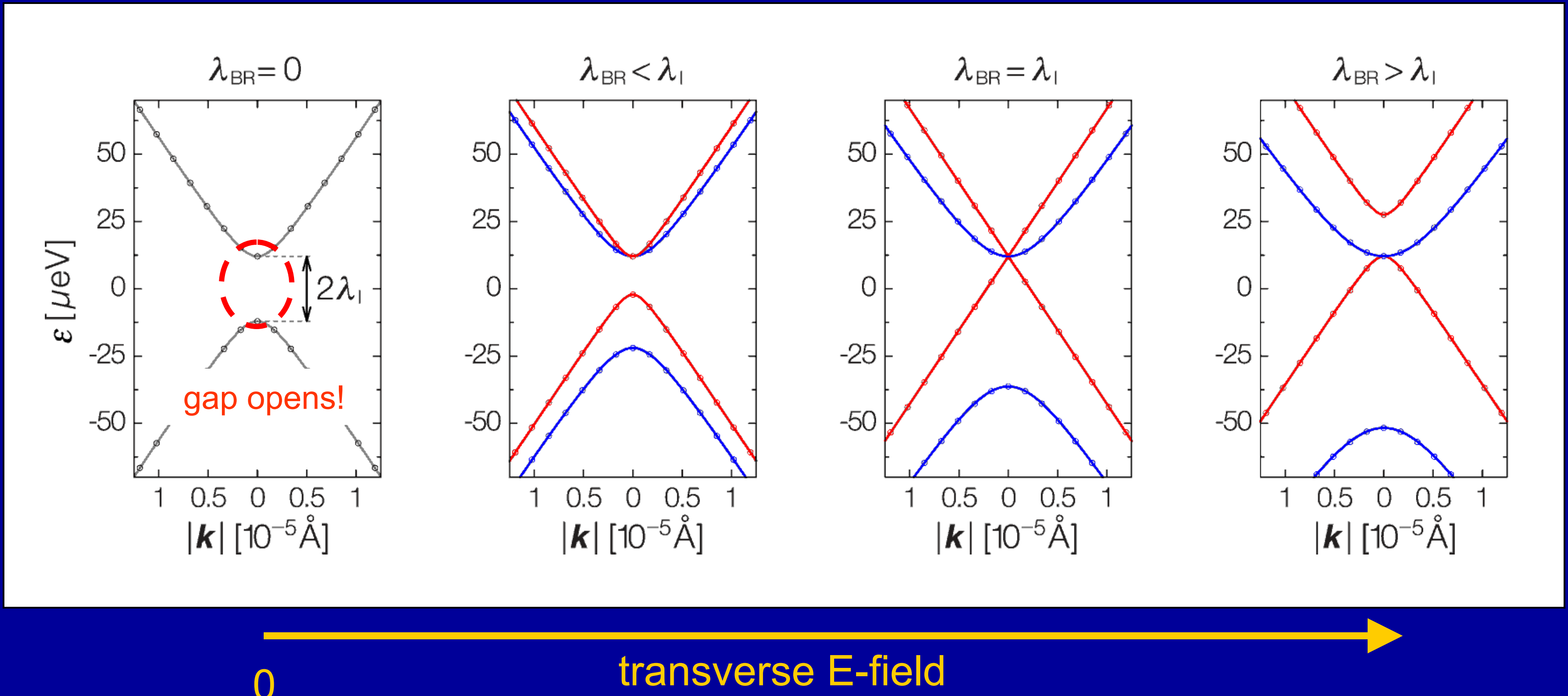
band-structure topologies in a transverse E-field

M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, Phys. Rev. B 80, 235431 (2009)
S. Konschuh, M. Gmitra, and J. Fabian, Phys. Rev. B 82, 245412 (2010)

Slonczewski, McClure & Yafet, Kane and Mele

$$H_I = \lambda_I \kappa \sigma_z s_z$$
$$H_{BR} = \lambda_{BR}(\kappa \sigma_x s_y - \sigma_y s_x)$$

$$E_{\mu\nu} = \mu\lambda_{BR} + \nu\sqrt{(\hbar v_F k)^2 + (\lambda_{BR} - \mu\lambda_I)^2}$$

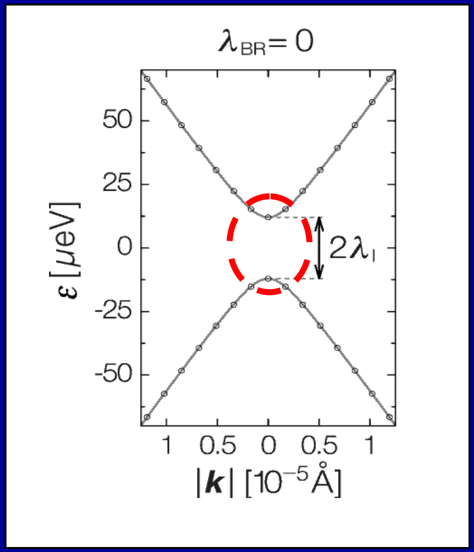


- LAPW Wien 2k
- self-consistent transverse electric field
- analytical description within 5% for ± 200 meV

:spin-orbit coupling in graphene at K:

the intrinsic gap puzzle

M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, Phys. Rev. B 80, 235431 (2009)



- our calculated gap is 24 micro eV
- previous calculations:

?

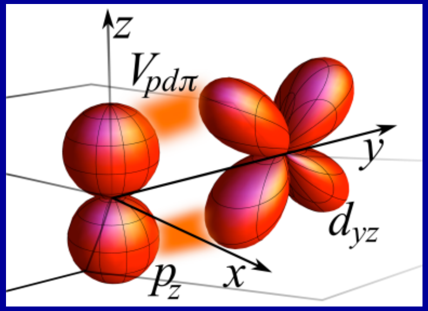
200 micro eV Kane and Mele, PRL 95, 226801 (2005)
1 micro eV Min et al, PRB 74, 165310 (2006)
1 micro eV Yao et al, PRB 75, 041401(R) (2007)
50 micro eV Boettger and Trickey, PRB 75, 121402(R) (2007)
25 micro eV (Jülich, S. Bihlmaier, private communication)
24.5 micro eV S. Abdelouahed et al, Phys. Rev. B 82, 125424 (2010)

TB
PP

all e

π-d mediated SOC

J. C. Slonczewski, PhD Thesis, Rutgers University, 1955
J. W. McClure and Y. Yafet, Proceedings of the Fifth Conference on Carbon, (Pergamon, 1962), Vol. 1, p 22.



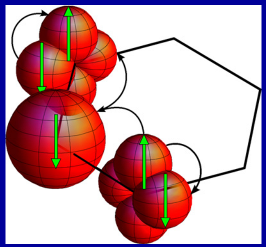
$$|p_z^A\rangle + i\gamma(\pm|d_{xz}^B\rangle \pm i|d_{yz}^B\rangle)$$

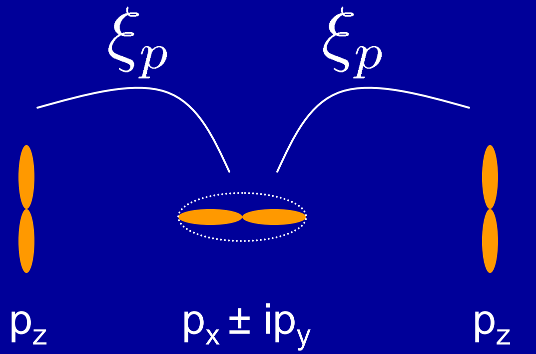
S. Konschuh, M. Gmitra, and J. Fabian, Phys. Rev. B 82, 245412 (2010)

S. Konschuh et al,
Phys. Rev. B 82, 245412 (2010)

σ-π mediated SOC

2nd order effect





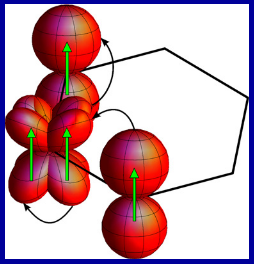
$\sim \xi_p^2$

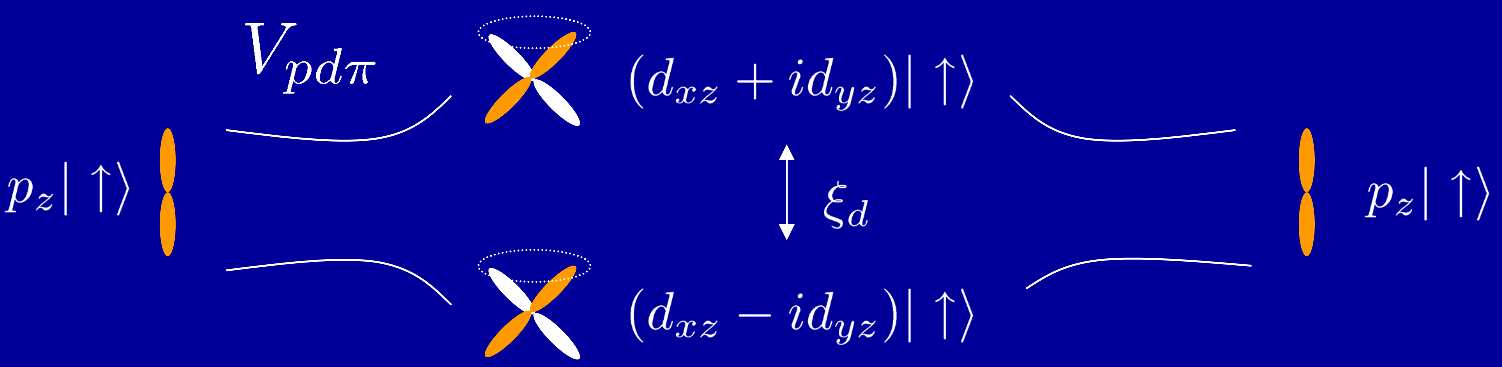
$$\langle p_z|\mathbf{L}|p_z\rangle = 0$$

$$\langle p_z|L_y|p_x\rangle \neq 0$$

π-d mediated SOC

1st order effect

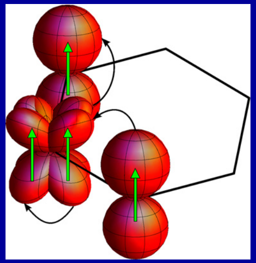


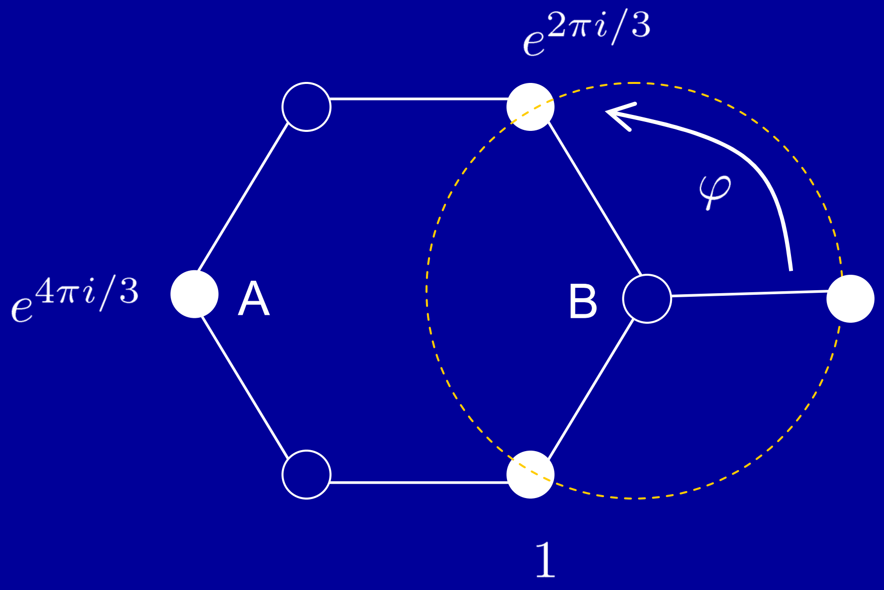


$\sim \xi_d$

why d orbitals?

symmetry at the K point





$$\overbrace{\vert p_z\rangle_A + \vert d_{xz} - i d_{yz}\rangle_B}^{f(r) z e^{-i\varphi}}$$

rotation about B by 120

$$[\vert p_z\rangle_A + \vert d_{xz} - i d_{yz}\rangle_B]\, e^{2\pi i/3}$$

$$[\vert p_z\rangle_B + \vert d_{xz} + i d_{yz}\rangle_A]\,\vert\uparrow\rangle \qquad [\vert p_z\rangle_A + \vert d_{xz} - i d_{yz}\rangle_A]\,\vert\downarrow\rangle$$

$$2\lambda_I$$

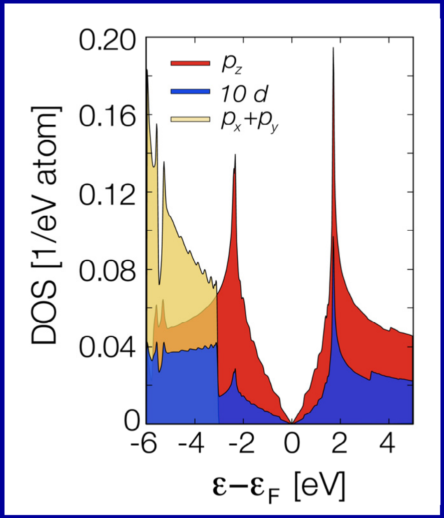
$$[\vert p_z\rangle_B + \vert d_{xz} + i d_{yz}\rangle_A]\,\vert\downarrow\rangle \qquad [\vert p_z\rangle_A + \vert d_{xz} - i d_{yz}\rangle_A]\,\vert\uparrow\rangle$$

J. W. McClure and Y. Yafet, Proceedings of the Fifth Conference on Carbon, (Pergamon, 1962), Vol. 1, p 22.

:spin-orbit coupling in graphene:

the intrinsic gap puzzle

M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, Phys. Rev. B 80, 235431 (2009)
S. Konschuh, M. Gmitra, and J. Fabian, Phys. Rev. B 82, 245412 (2010)



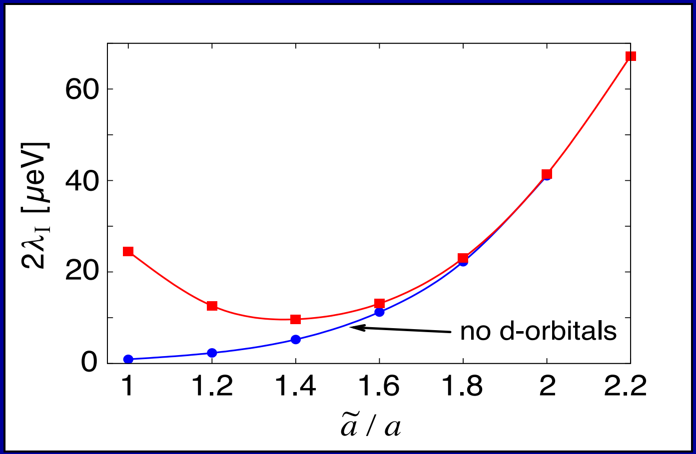
The intrinsic gap is 96% from d and higher orbitals!!!

$$2\lambda_I = \frac{4(\epsilon_p - \epsilon_s)}{9V_{sp\sigma}^2}\xi_p^2 + \frac{9V_{pd\pi}^2}{(\epsilon_d - \epsilon_p)^2}\xi_d$$

σ- π SOC: 1 μeV
irrelevant

π-d SOC: 23 μeV
dominates

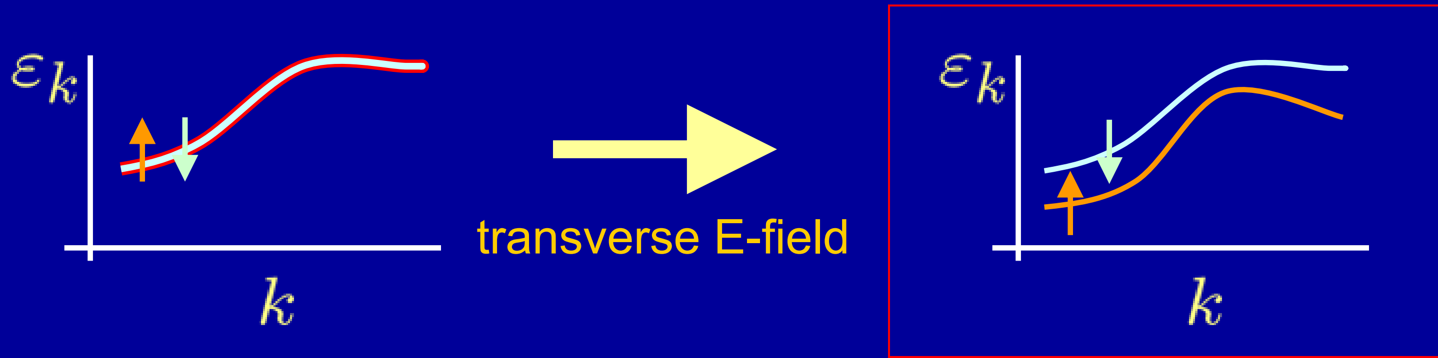
intrinsic gap versus strain
also confirms the picture:



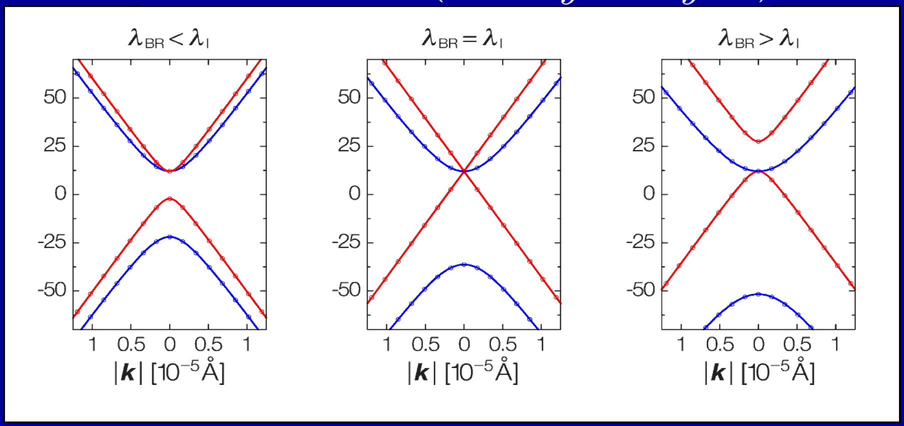
:spin-orbit coupling in graphene:

extrinsic (Bychkov-Rashba) coupling

M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, Phys. Rev. B 80, 235431 (2009)
S. Konschuh, M. Gmitra, and J. Fabian, Phys. Rev. B 82, 245412 (2010)



$$H_I = \lambda_I \kappa \sigma_z s_z$$
$$H_{BR} = \lambda_{BR}(\kappa \sigma_x s_y - \sigma_y s_x)$$



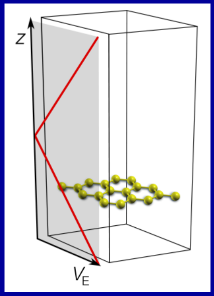
σ-π mediated Stark effect + SOC

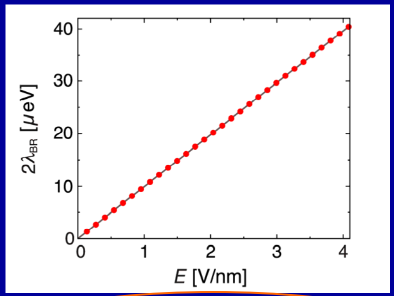
$$\lambda_{BR} = \frac{eEz_{sp}}{3V_{sp\sigma}}\xi_p + \sqrt{3}\frac{eEz_{pd}}{(\epsilon_d - \epsilon_p)}\frac{3V_{pd\pi}}{(\epsilon_d - \epsilon_p)}\xi_d$$

σ- π SOC dominates

π-d SOC irrelevant

Min et al, PRB 74, 165310 (2006)



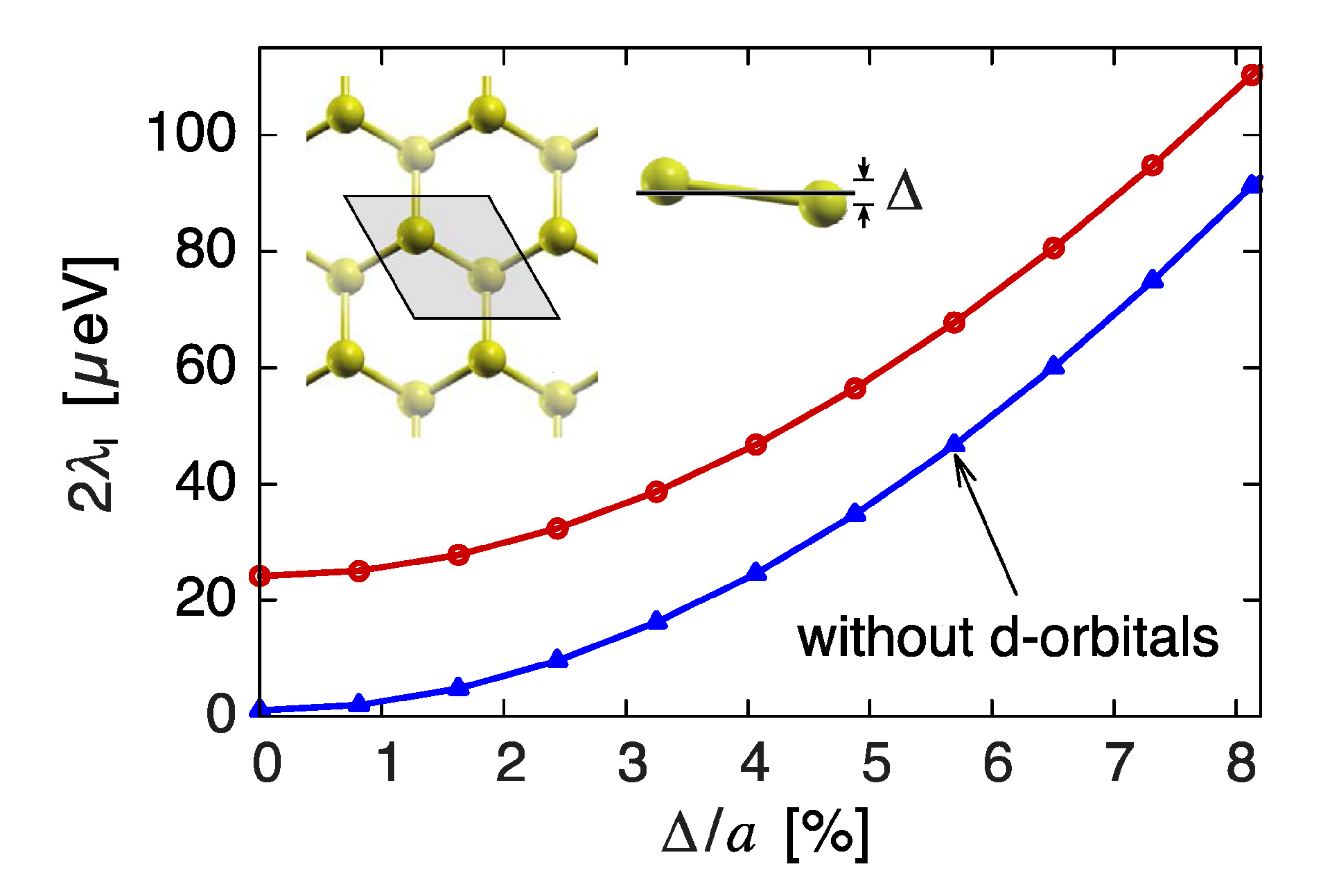


10 μeV per V/nm

:buckling of graphene:

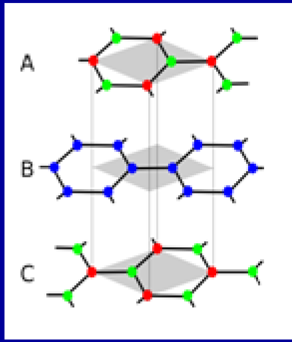
sigma-pi coupling

M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, Phys. Rev. B 80, 235431 (2009)



:outline:

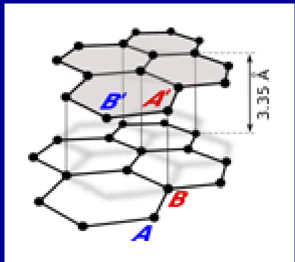
- bilayer, trilayer, and graphite



Order-of-magnitude increase SOC due to interlayer hopping?

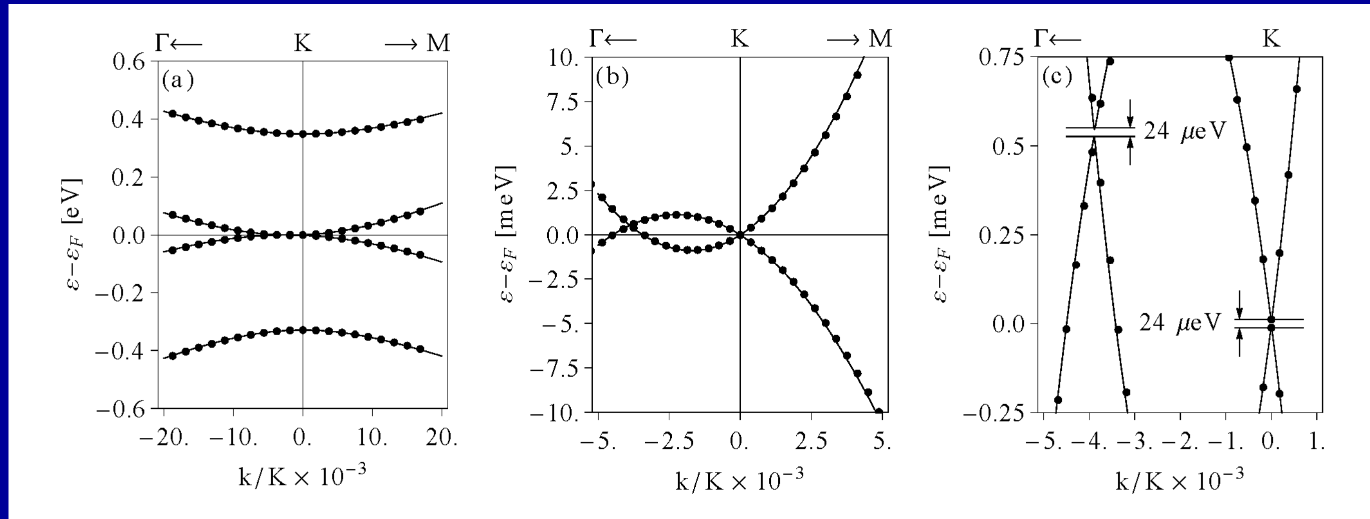
F. Guinea, New J. Phys. 12, 083063 (2010)
E. McCann and M. Koshino, Phys. Rev. B 81, 241409(R) (2010)

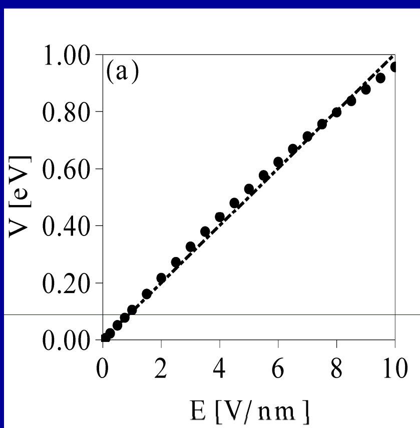
:AB bilayer:



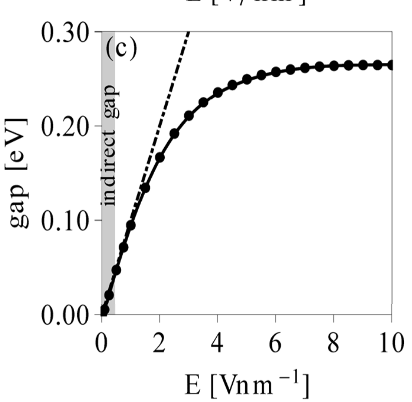
Wien2k and tight binding

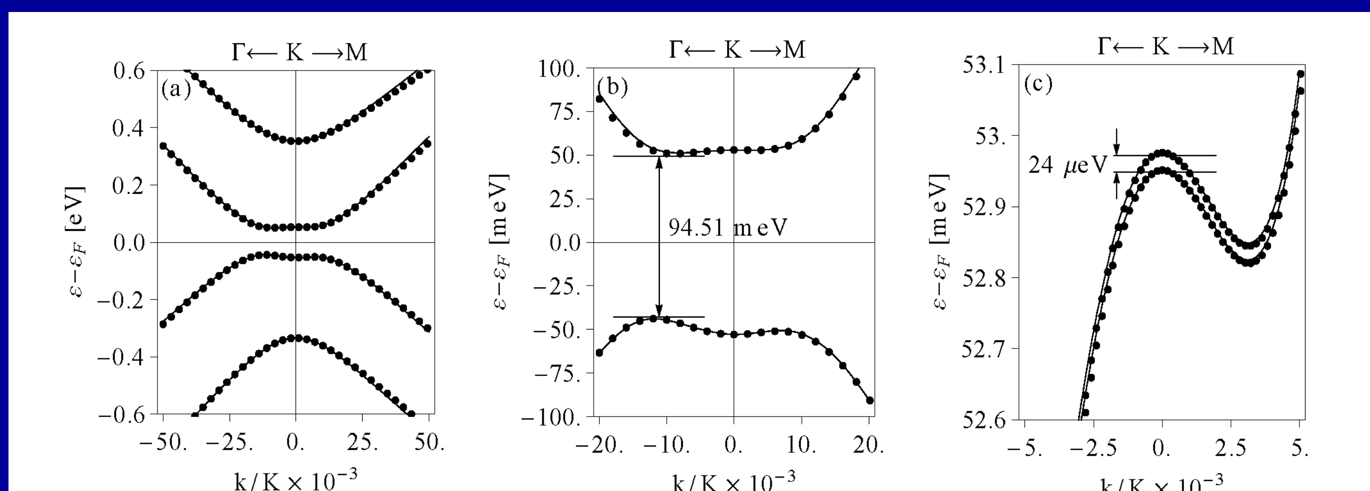
E=0



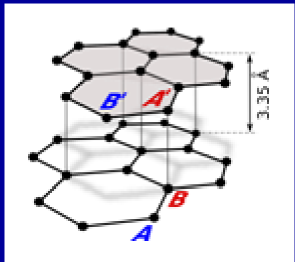


E=1 V/nm





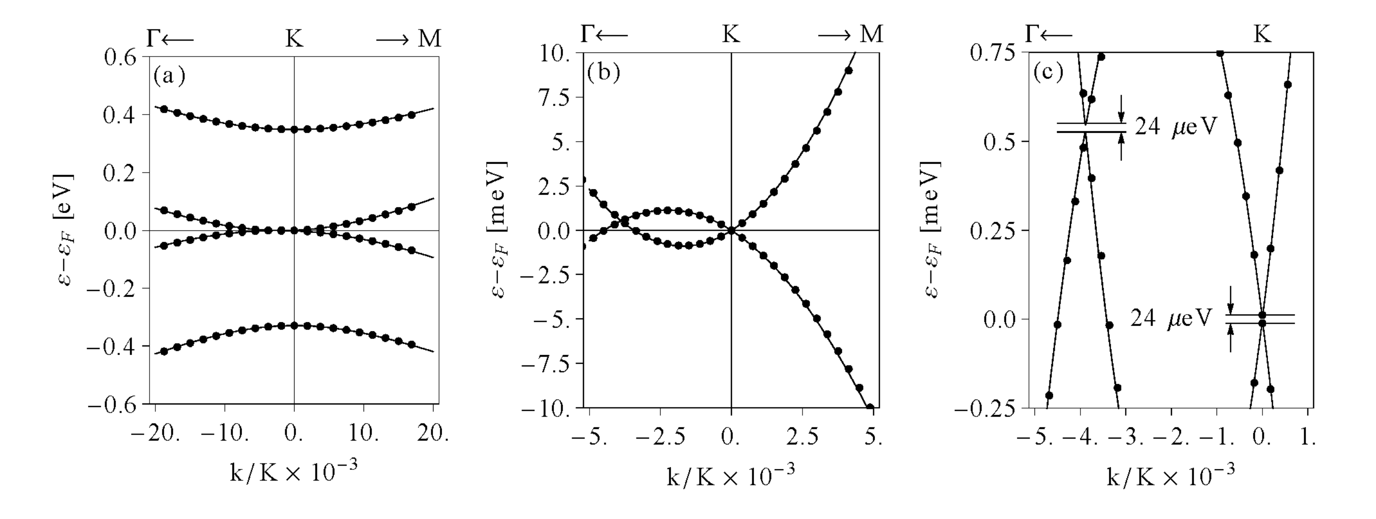
Extrinsic splitting given by intrinsic value!!!

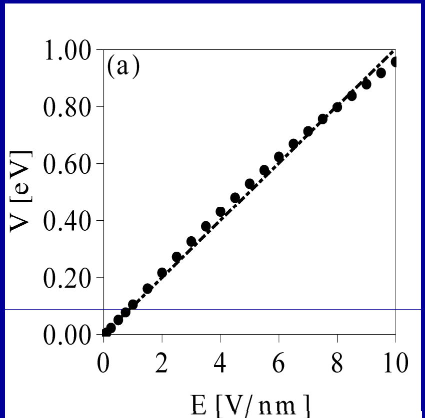


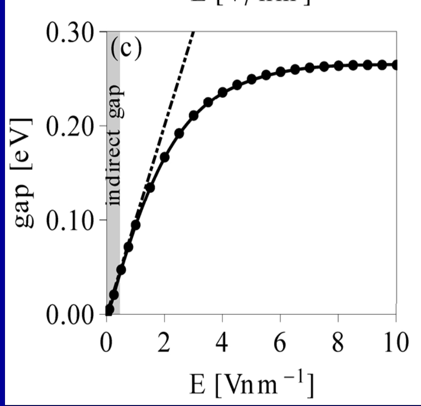
:AB bilayer:

Wien2k and tight binding

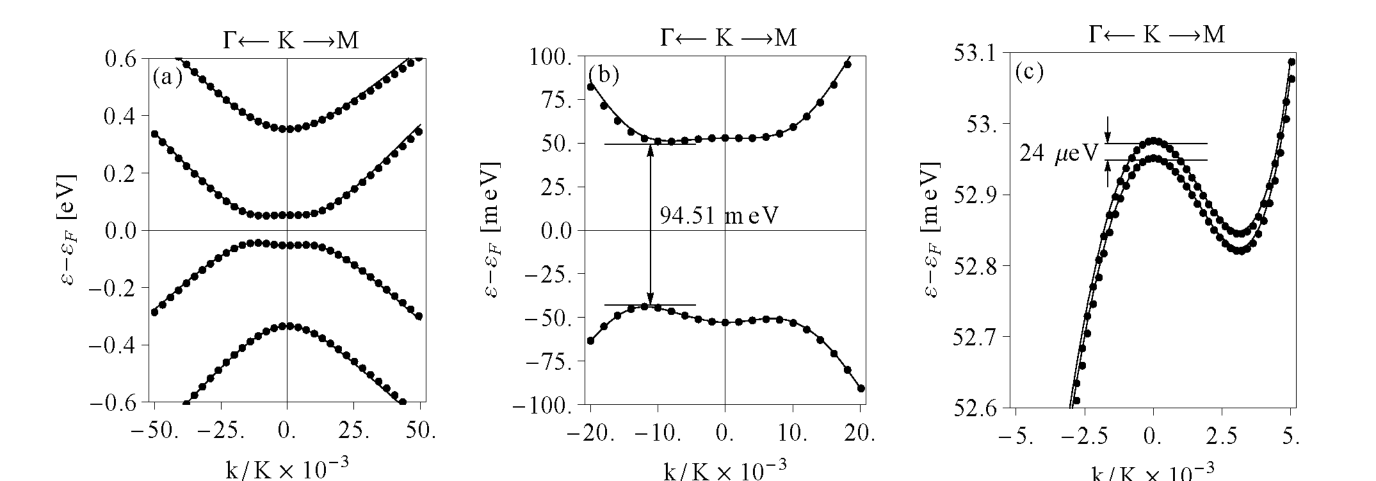
E=0



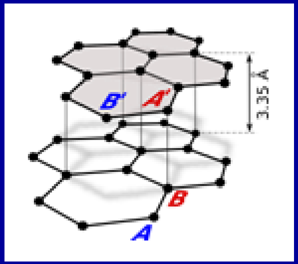




E=1 V/nm



Extrinsic splitting given by intrinsic value!!!



:Hamiltonian for AB bilayer:

S. Konschuh, M. Gmitra, D. Kochan, and J. Fabian,
Theory of spin-orbit coupling in bilayer graphene, arXiv: 1111.7223

Intrinsic: F. Guinea, New J. Phys. 12, 083063 (2010)

$$H_{\mathrm{SOC}} = H_{\mathrm{I}} + H_{\mathrm{BR}} + H_{\mathrm{inter}} + H_{\mathrm{el}}$$

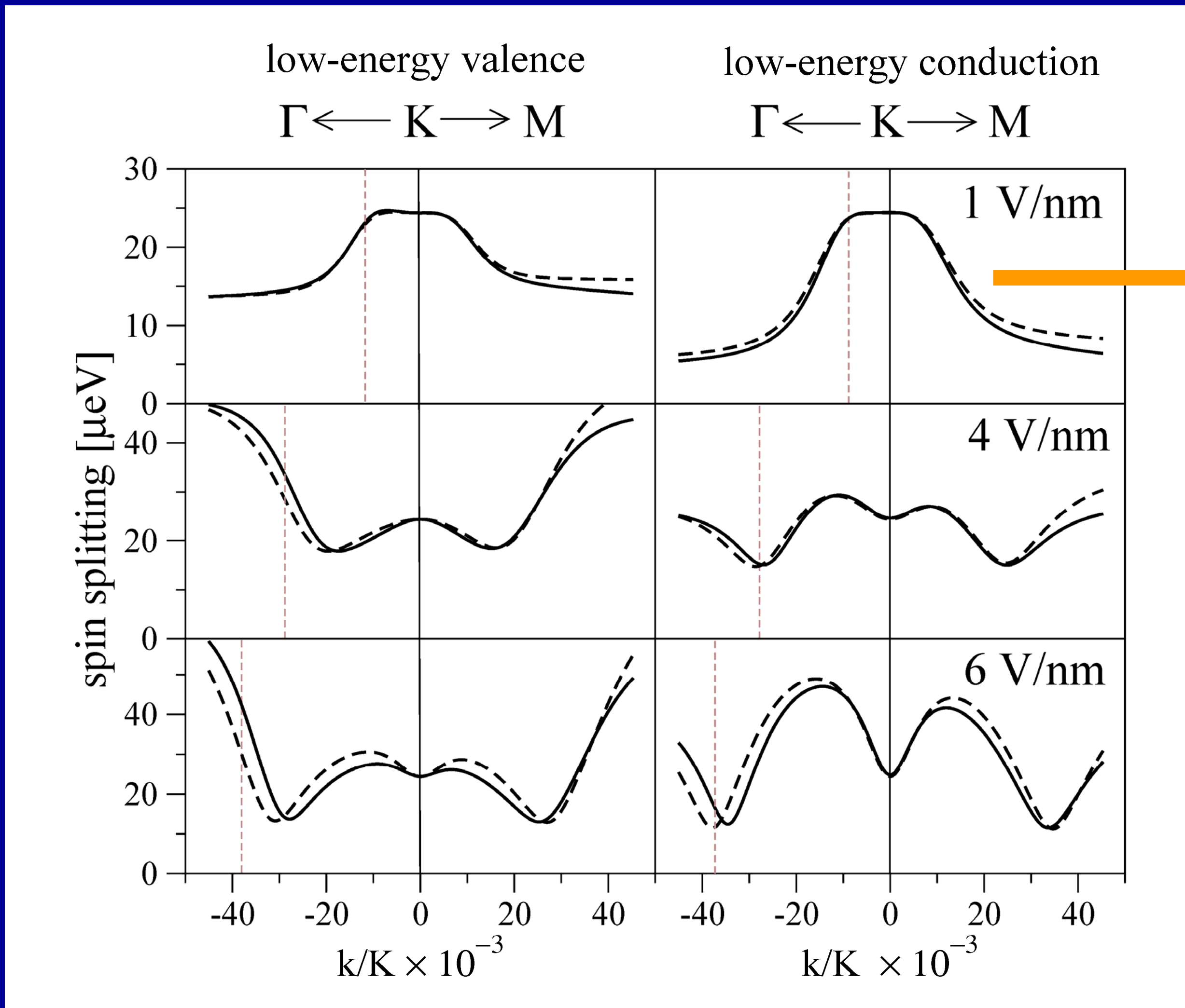
$$H_{\mathrm{I}} = \tfrac{1}{2}\left[(\Delta_{\mathrm{I}} - \Delta'_{\mathrm{I}})\sigma_0 + (\lambda_{\mathrm{I}} + \lambda'_{\mathrm{I}})\sigma_z\right]\mu_0\tau s_z + \tfrac{1}{2}\left[(\Delta_{\mathrm{I}} + \Delta'_{\mathrm{I}})\sigma_0 + (\lambda_{\mathrm{I}} - \lambda'_{\mathrm{I}})\sigma_z\right]\mu_z\tau s_z\,,$$

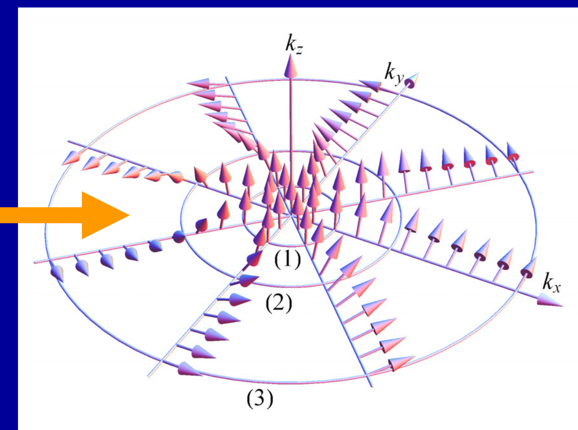
$$H_{\mathrm{BR}} = \tfrac{1}{2}(\lambda_{0-}\,\mu_0 + \lambda_{0+}\,\mu_z)(\tau\sigma_x s_y - \sigma_y s_x)\,,$$

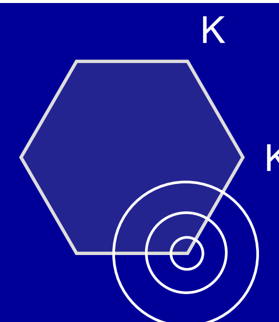
$$H_{\mathrm{inter}} = -\tfrac{1}{2}(\lambda_{4+}\,\sigma_z + \lambda_{4-}\,\sigma_0)(\tau\mu_x s_y + \mu_y s_x)\,,$$

$$H_{\mathrm{el}} = \tfrac{\lambda_1}{2} s_z(\mu_x\sigma_x - \mu_y\tau\sigma_y) + \tfrac{\lambda_3}{4}\left[\mu_x(\tau\sigma_x s_y + \sigma_y s_x) + \mu_y(\tau\sigma_y s_y - \sigma_x s_x)\right].$$

:spin splittings in AB bilayer:

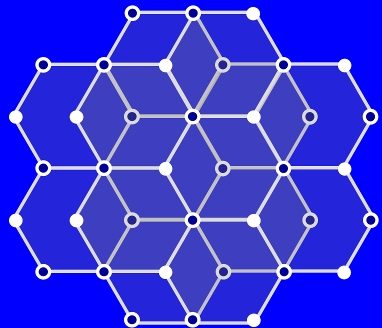






:graphite:

Wien2k



c=3.355 (6.71) Å