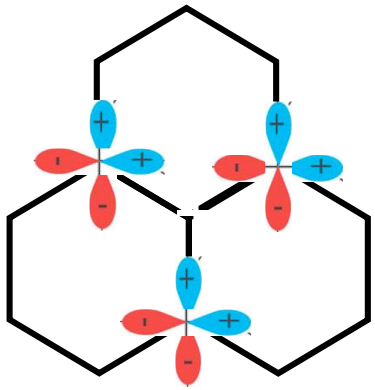
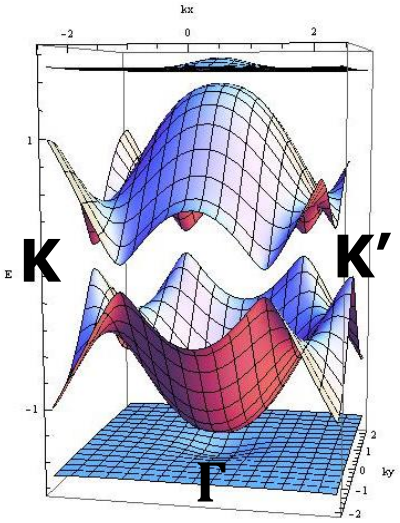
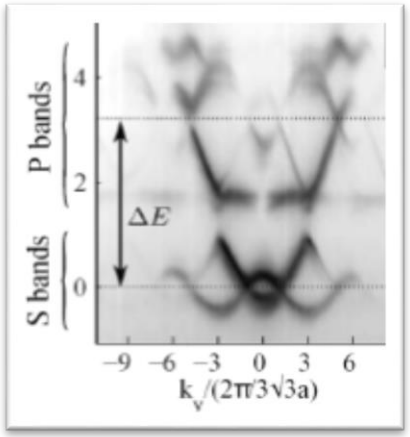
Orbital-active honeycomb materials

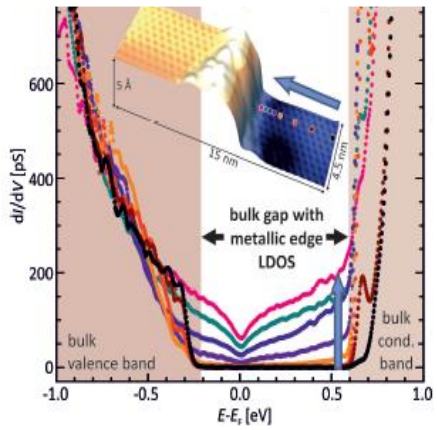
Congjun Wu

Department of Physics, UC San Diego







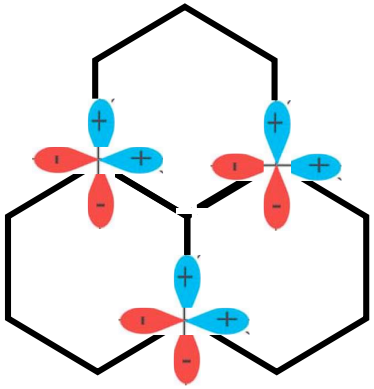


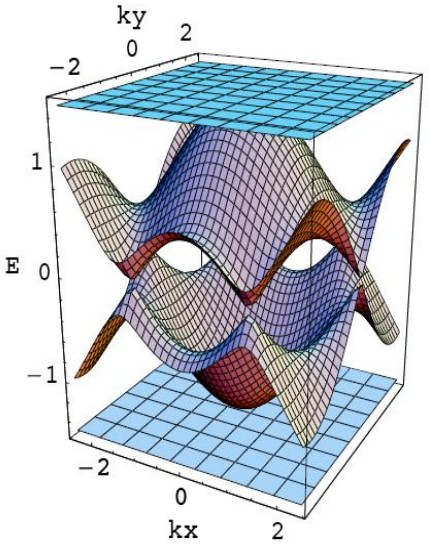
Berkeley, 04/30/2019

Collaborators

Yi Li	(UCSD →Princeton→ Johns Hopkins)
Gufeng Zhang	(UCSD → experiment)
Shenglong Xu	(UCSD → Univ. Maryland)
S. Das Sarma	(University of Maryland)
L. Balents	(UCSB)
Chuanwei Zhang	(Washington state → UT Dallas)
Gang Li	(Shanghai Tech.)
Werner Hanke	(Wuerzburg Univ.)

Flat band: Wigner crystal, ferromagnetism





Orbital-active honeycomb

$(p_x p_y)$, (d_{xz}, d_{yz})

$(d_{r^2-z^2}, d_{x^2-y^2})$

- Large gap topo-insulator
- Frustrated orbital exchange -120° model
- f-wave supercond.

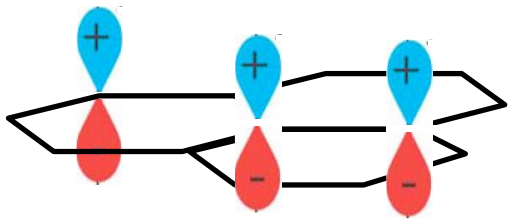
- Bismuthene, Stanene
- Polariton lattice
- Twisted bilayer graphene
- transition metal oxides

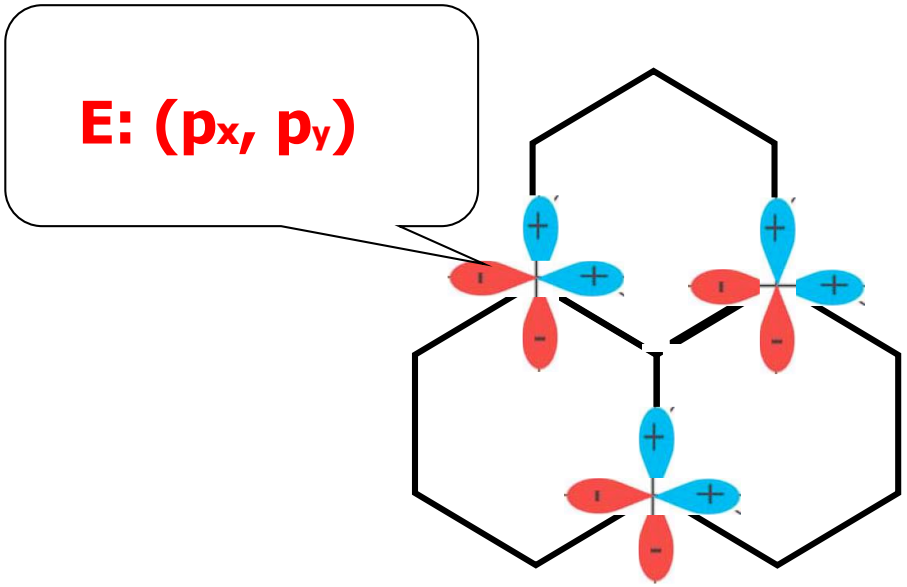
The dual version (p_x, p_y) to graphene (p_z)

Orbital-inactive

Orbital-active: degeneracy

A_2 (p_z) graphene





Recent foci:

bilayer twisted graphene (Paballo),

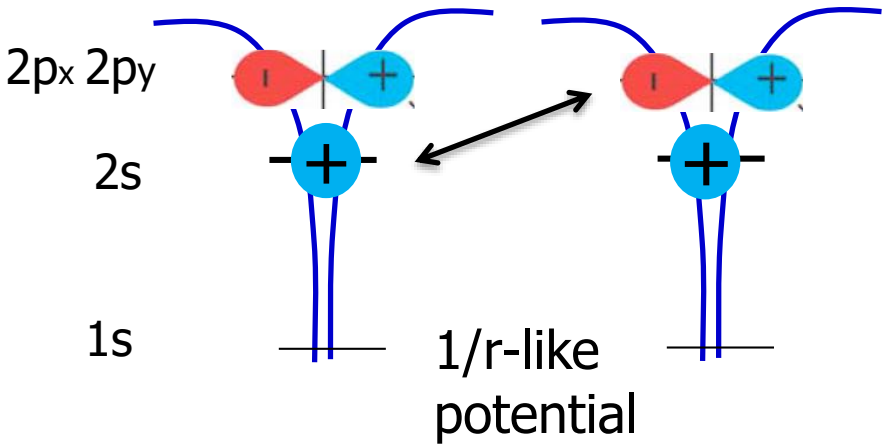
trilayer graphene: gate tunable Mott states (Feng Wang)

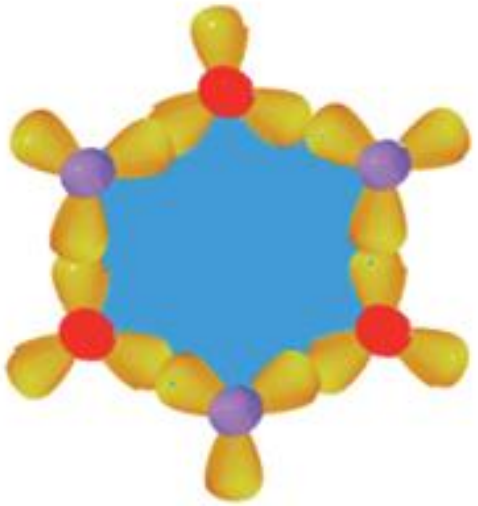
How to find orbital-active honeycomb system?

- Graphene is not orbital-acitive

sp_2-hybridization → $2s$, $2p_x$, $2p_y$, strong σ -bonds.

σ -bands away from Fermi surface.

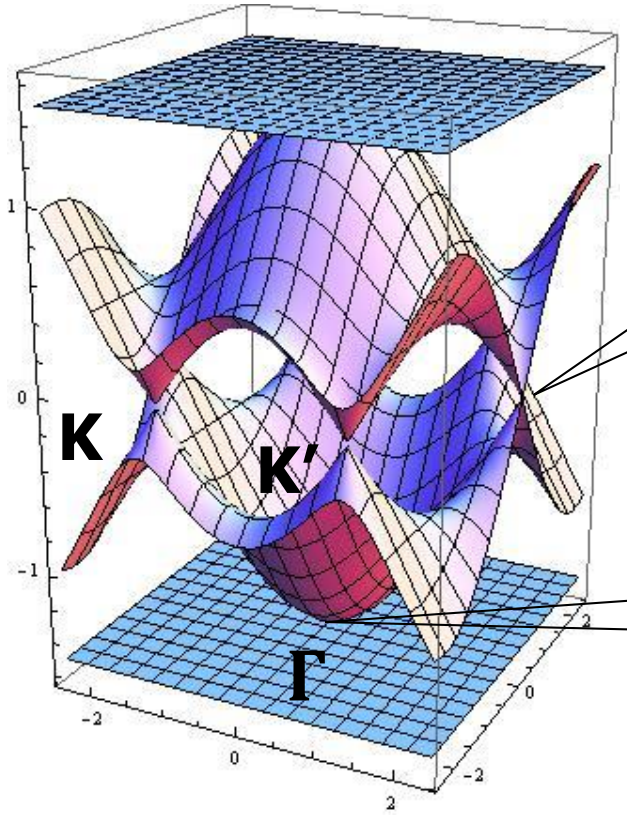




- Need to passivate the s and p_z-orbitals.

Flat band and Dirac cones (orbital-enriched)

C. Wu, D. Bergman, L. Balents, and S. Das Sarma, PRL 99, 70401 (2007).
C. Wu, PRL 101, 186107 (2008).



Dirac cones: orbital structure → large gap topo-insulator

W. C. Lee, C. Wu, S. Das Sarma, PRA 2010;
G.F. Zhang, Y. Li, C. Wu, PRB 90 (2014).

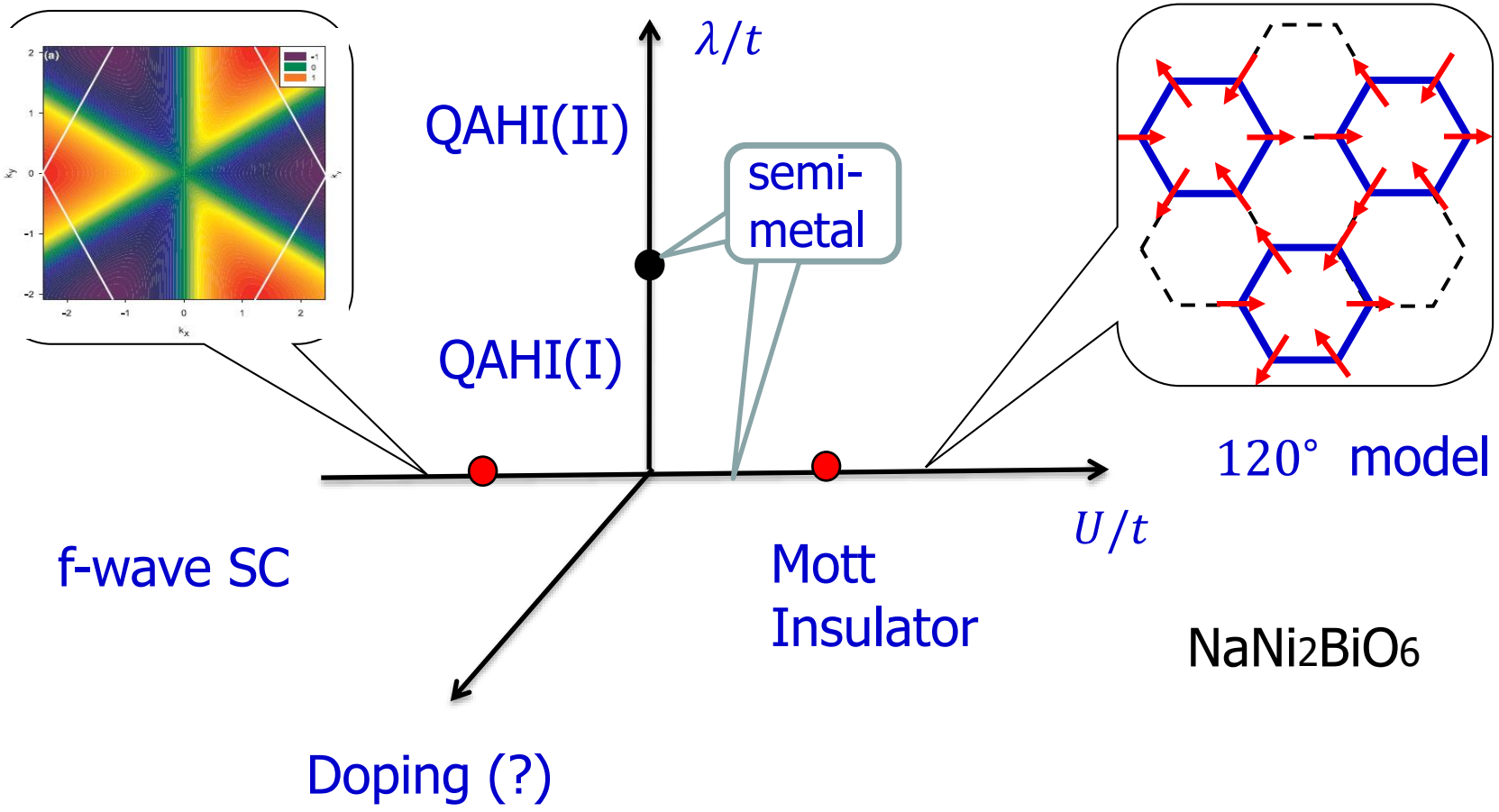
Flat band → ferromagnetism, Wigner crystal

S. Z. Zhang, H. h. Hung, C. Wu, PRA 82, 053818 (2010).

Topology and frustration

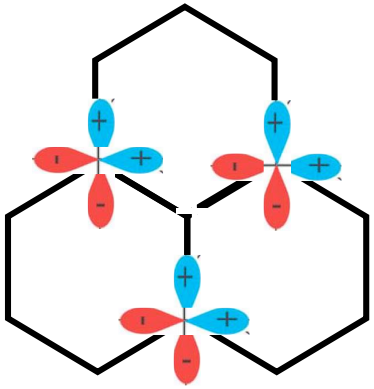
Lee, CW, Das Sarma, PRA (2010).

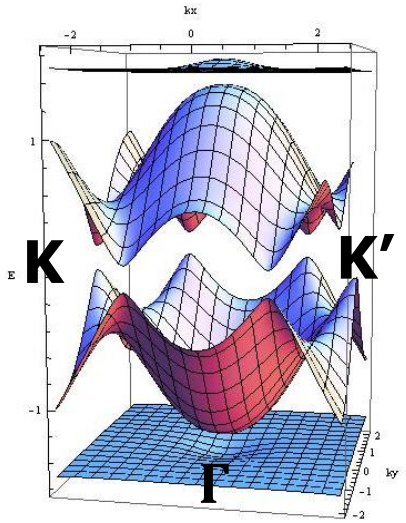
CW, PRL.100, 200406 (2008).



arxiv1807.02528, Cava, Broholm et al.

Flat band: Wigner crystal, ferromagnetism





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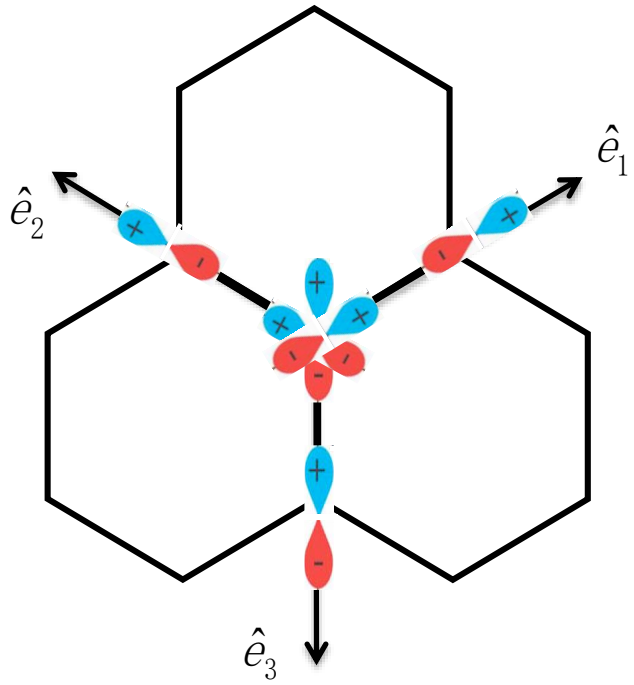
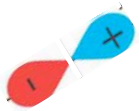
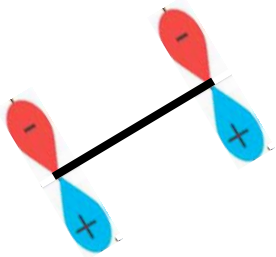
Minimal Hamiltonian (σ -bonding)

$$H_t = t_{//}\Big\{ \sum_{\vec{r}\in A} [p_1^+(\vec{r})p_1(\vec{r}+\hat{e}_1) + h.c.\,] + [p_2^+(\vec{r})p_2(\vec{r}+\hat{e}_2) + h.c] + [p_3^+(\vec{r})p_3(\vec{r}+\hat{e}_3) + h.c] \Big\}$$





$$p_1 = \frac{\sqrt{3}}{2}p_x + \frac{1}{2}p_y \qquad p_2 = -\frac{\sqrt{3}}{2}p_x + \frac{1}{2}p_y \qquad p_3 = -p_y$$

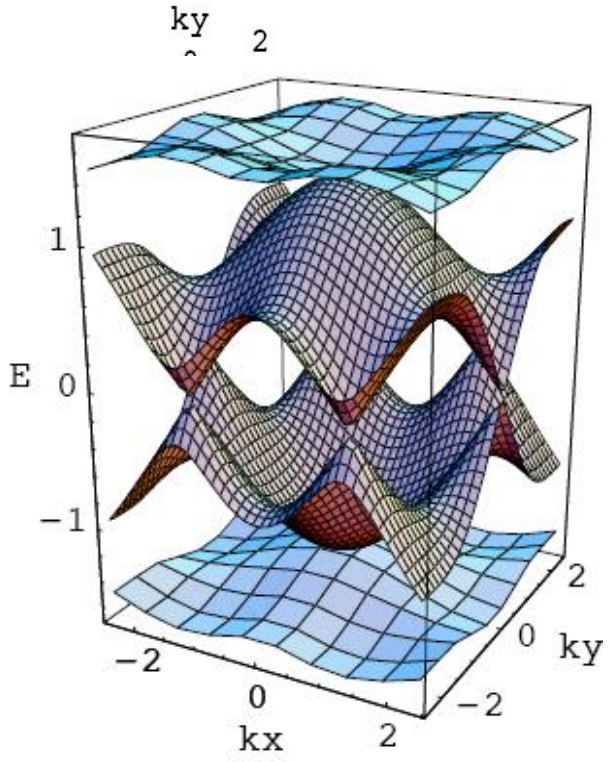


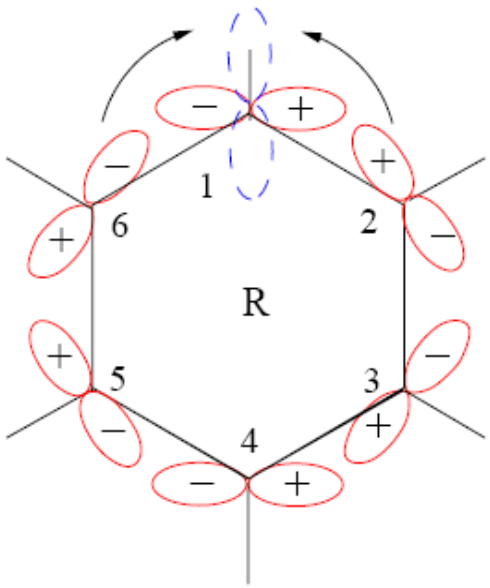
- π-bonding neglected – good approx. in transition metal oxide. Not good in semiconductor.

$t_\perp$ **π-bond**

C. Wu, D. Bergman, L. Balents, and S. Das Sarma, PRL 99, 70401 (2007)

Flat bands -- **localized** eigenstates

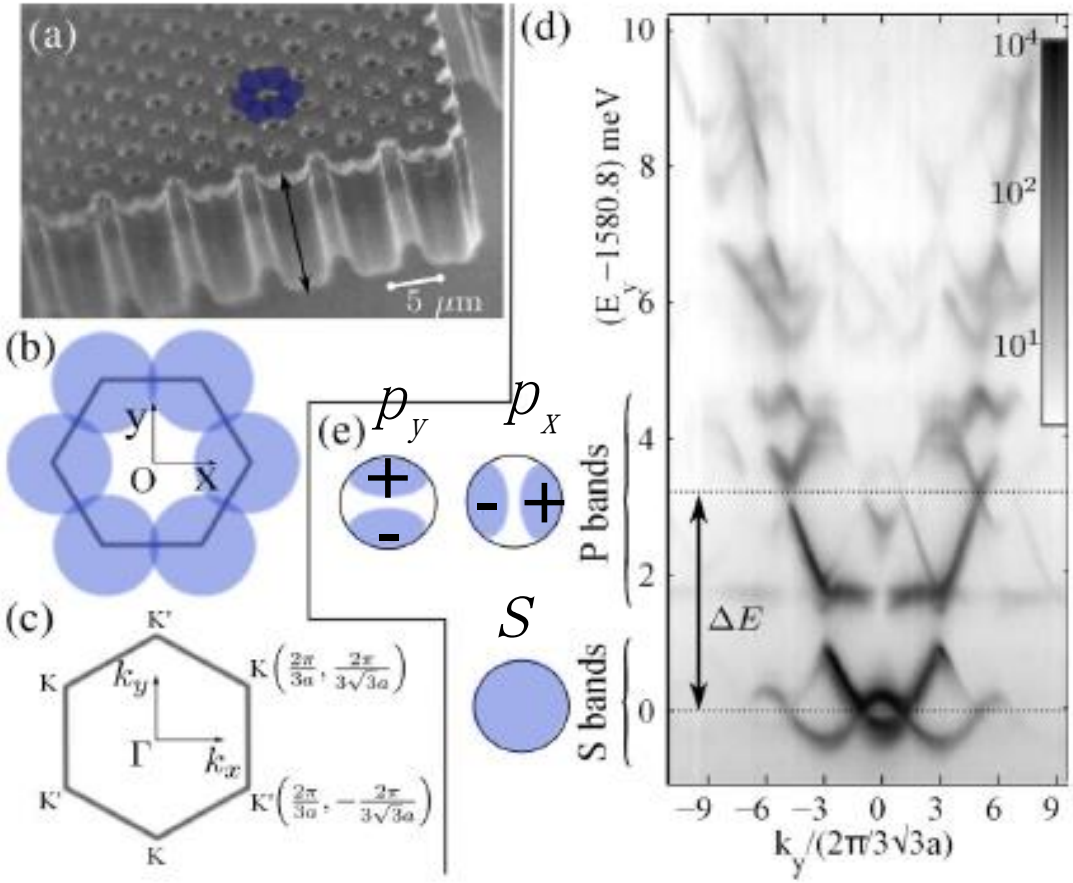




C. Wu, D. Bergman, L. Balents, and S. Das Sarma, PRL 99, 70401 (2007).

- If $t_\perp$ is included, flat bands → narrow bands .

Observed! (polariton in the p_x-p_y bands of the honeycomb lattice)

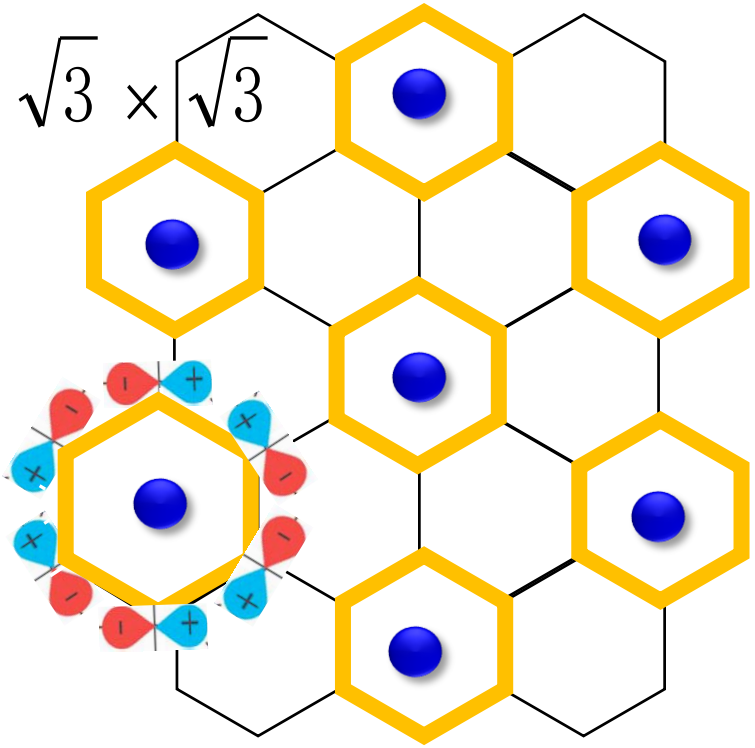


"Direct Observation of Dirac Cones and a flatband in a honeycomb lattice for Polaritons",

T. Jacqmin, I. Carusotto, et al. PRL 112, 116402 (2014)

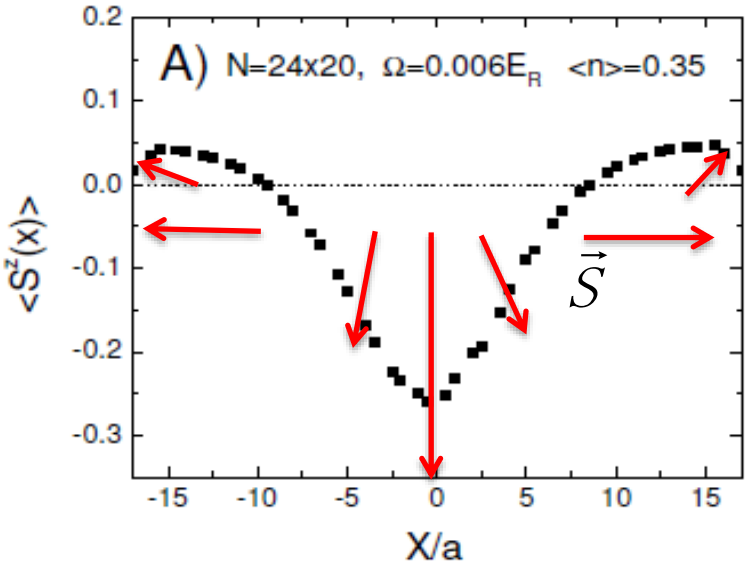
Strong correlations in the flat-band

- Wigner crystal (spinless fermions or bosons).



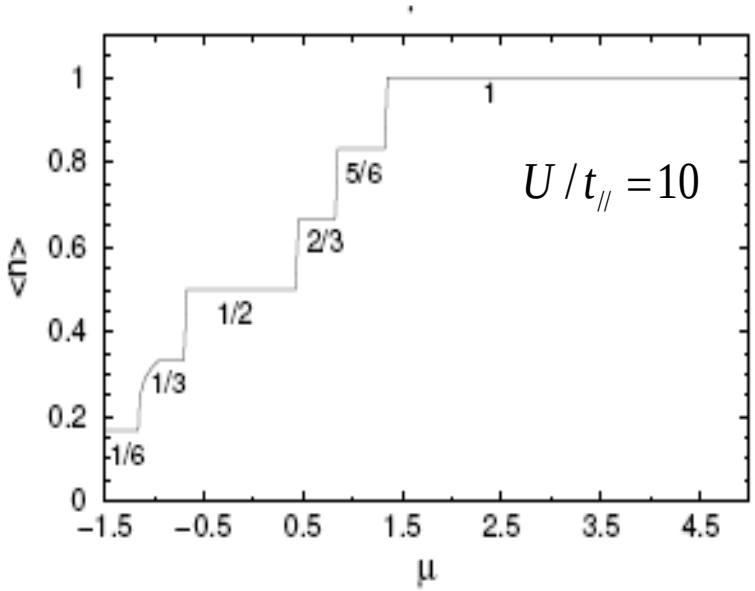
C. Wu, D. Bergman, L. Balents, and S. Das Sarma, PRL 99, 70401 (2007).

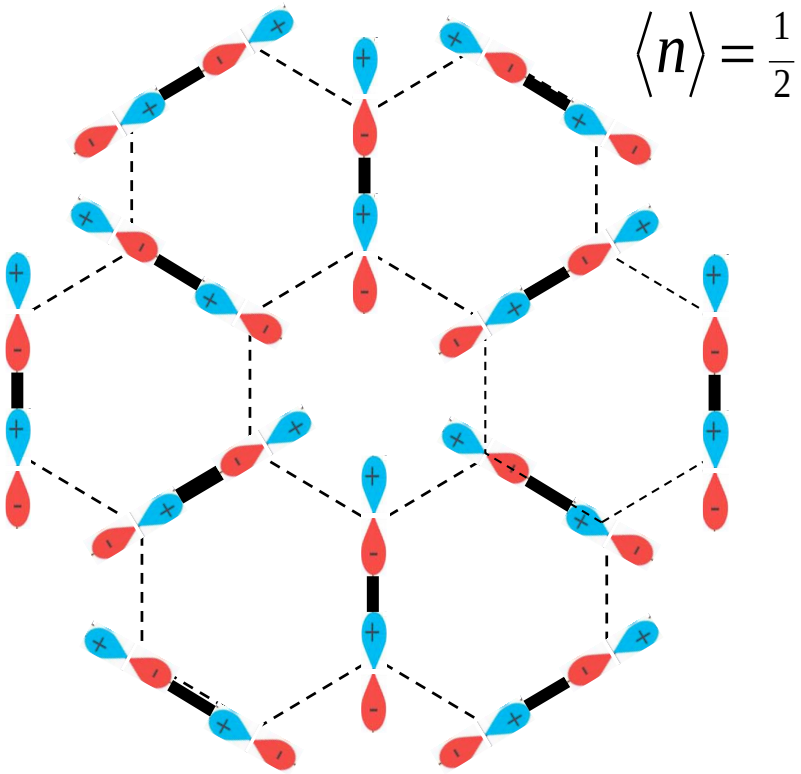
- **Flat-band FM** for spinful fermions.
- Large entropy → good for cold atom expt.
- Skyrmion texture.



S. Z. Zhang, H. h. Hung, C. Wu, PRA 82, 053818 (2010).

Orbital ordering with strong repulsions

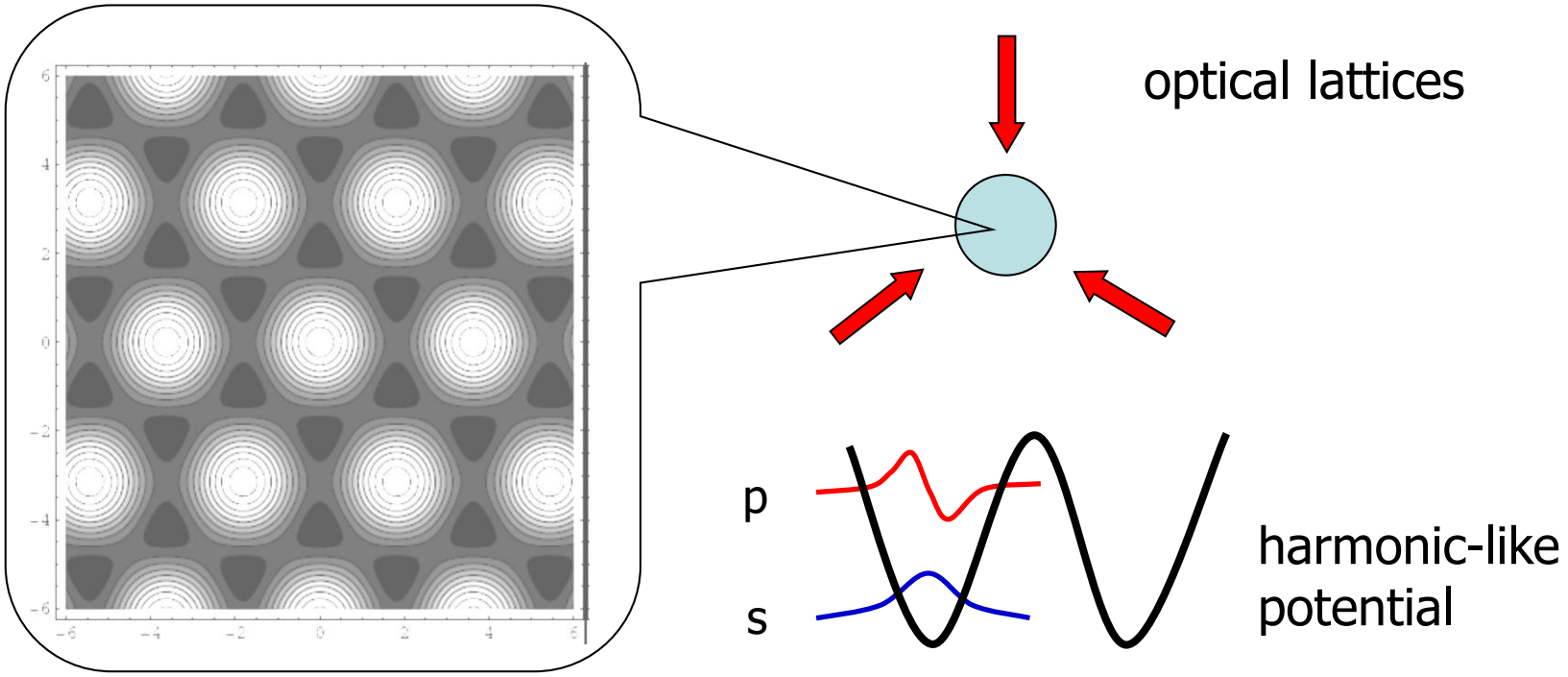




- Various orbital ordering insulating states at commensurate fillings.

Kekule pattern

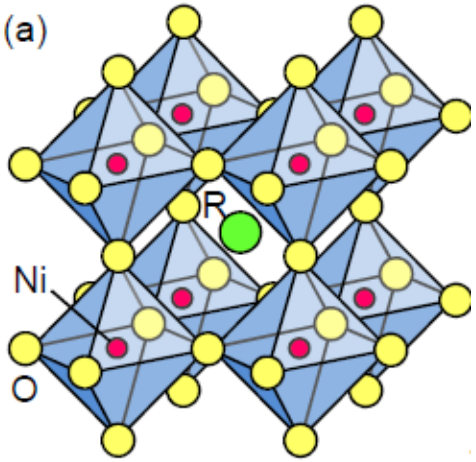
How to make p_x /p_y -orbital active?

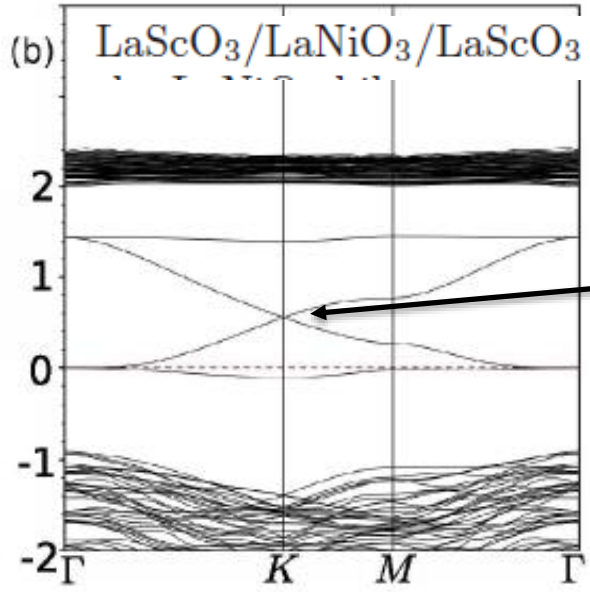


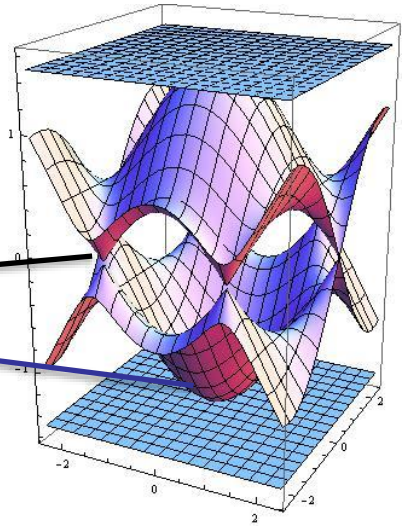
- p_x /p_y-orbital bands well separated from *s*.
- Strong confinement along z-direction → pz pushed to high energy

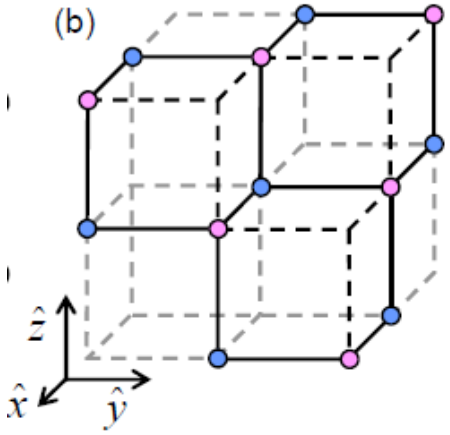
G. Grynberg et al., Phys. Rev. Lett. **70**, 2249 (1993).
also recent works from K. Sengstock, Esslinger, Bloch's groups.

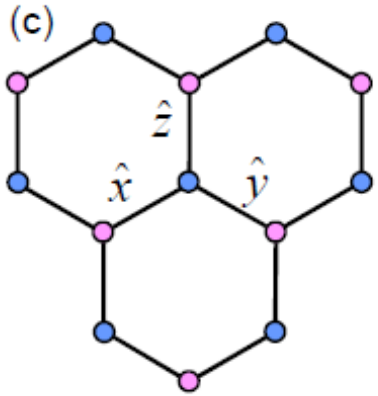
Transition metal oxide bilayer (111) LaNiO3









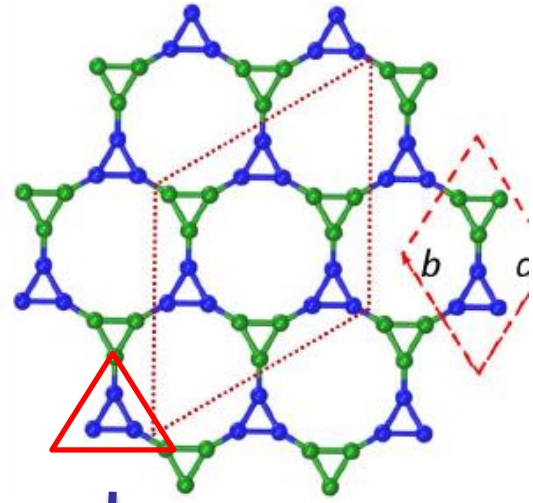


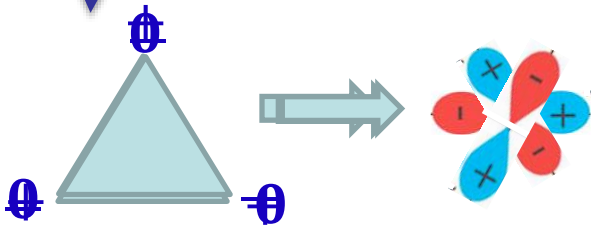
e_g : 2d rep

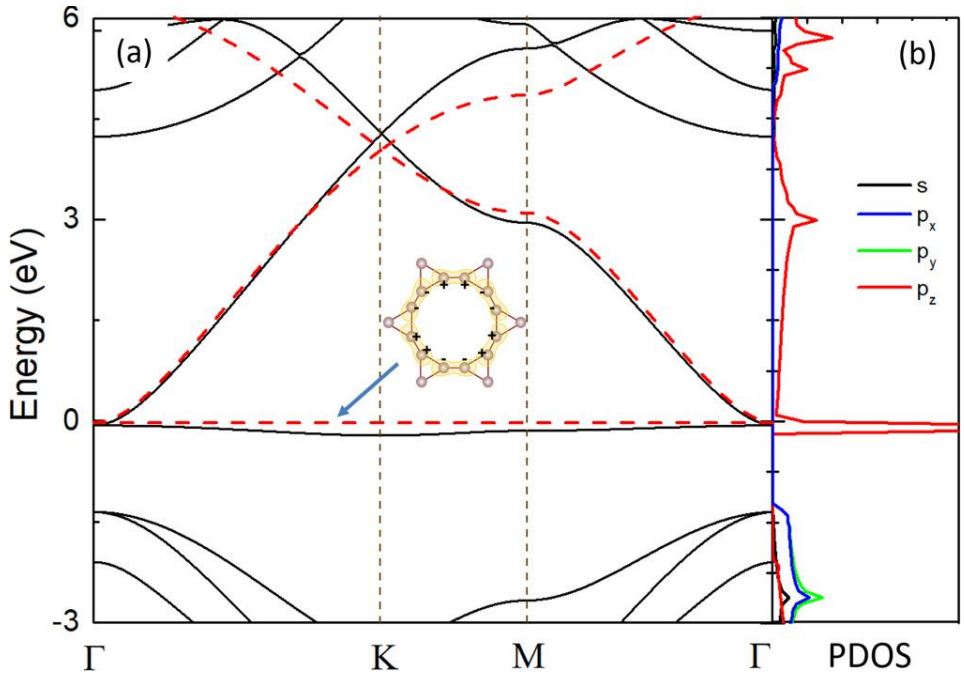
$d_{r^2-3z^2}$,
$d_{x^2-y^2}$

D. Xiao, et,al., Nat.Comm. (2011); Ying Ran, et al, PRB, (2011).

Flat-band in "Kagome graphene"





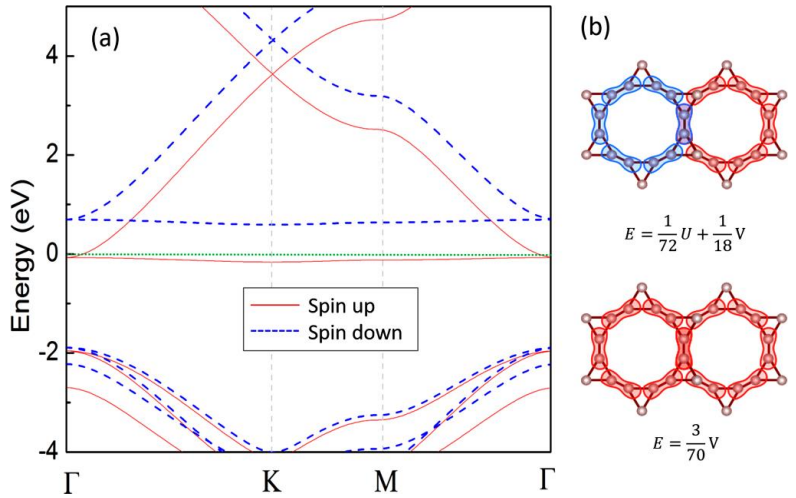


Y. P. Chen, S. L. Xu, Y. Xie, C. Zhong, **CW**, S. B. Zhang, PRB 98,035135 (2018).

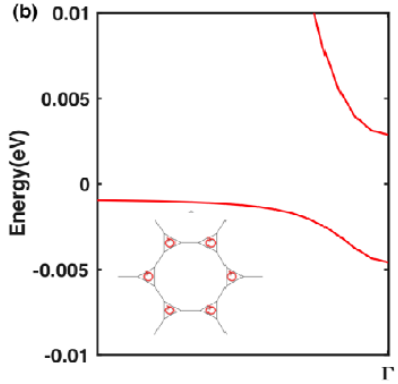
Ferromagnetism and spontaneous quantum anomalous Hall state

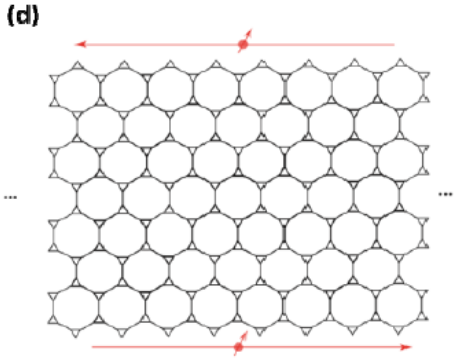
LDA: dope holes:
half-filled flat-band

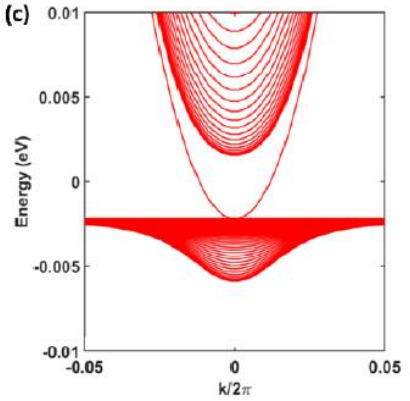
Y. P. Chen, S. L. Xu, Y. Xie, C. Zhong, **CW**, S. B. Zhang, PRB 98,035135 (2018).



Mean-field: Spontaneous generation of orbital moment $\langle L_z \rangle = 0.004\hbar$

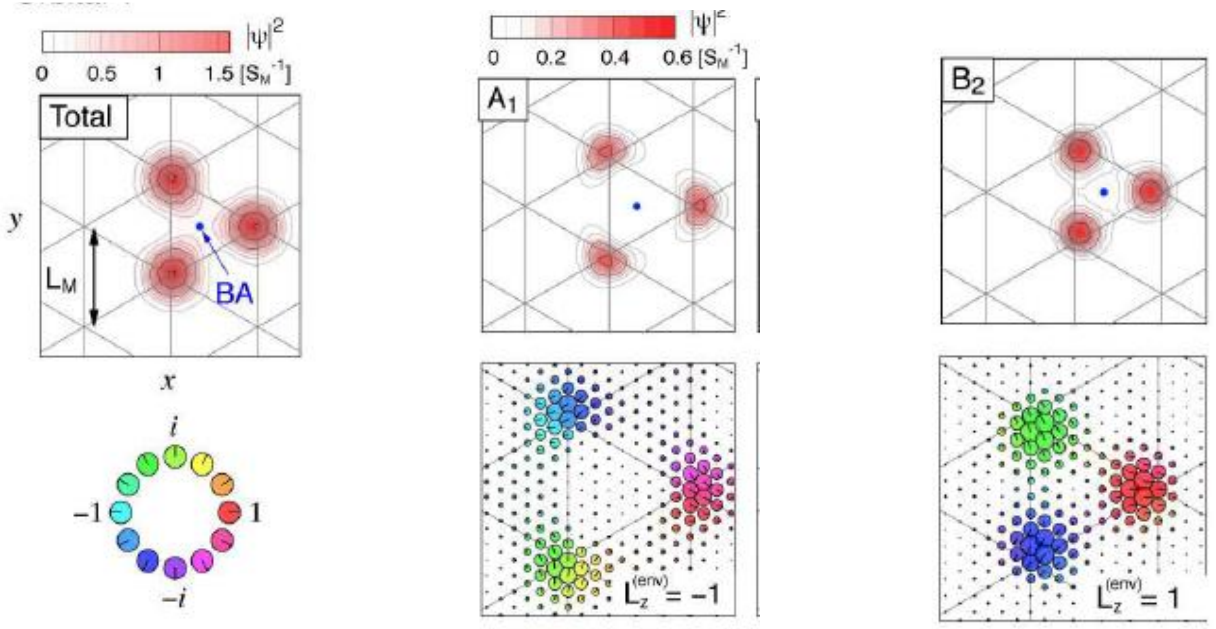




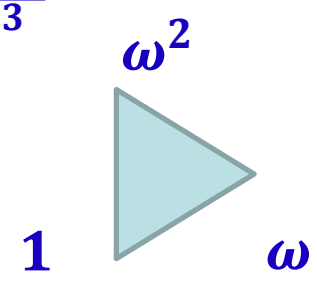


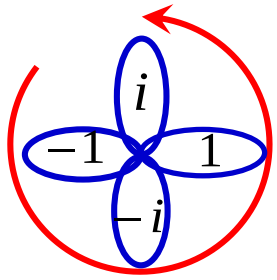
Sun, Yao, Fradkin, Kivelson, PRL 2009

Wannier orbitals in twisted bilayer graphene



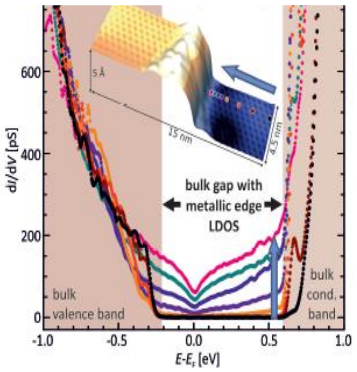
$$\omega = e^{\frac{i2\pi}{3}}$$

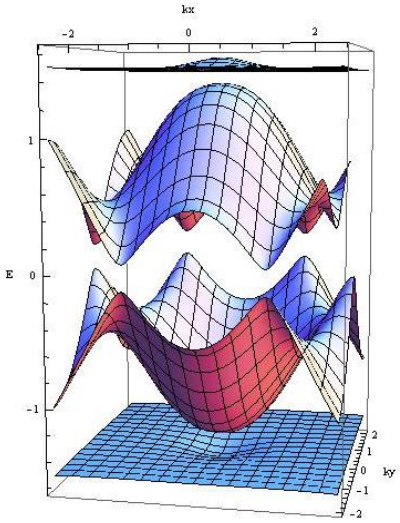




Liang Fu et al, PRX 8, 031087 (2018).

large topo-gap at the atomic SO energy scale





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- FM , Wigner crystal in flat band
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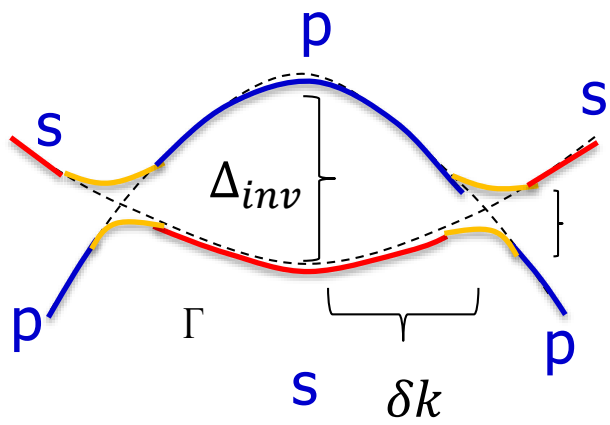
- f-wave supercond.

sp -band inversion -- small gap

- HgTe/HgCdTe: **s-p hybridization.**

Bernevig, Hughs, Zhang Science 314, 1757 (2006); Molenkamp's group, Science. 318 766–770 (2007)



$$\Delta_{topo}/\Delta_{inv} \propto \delta k a_0$$

$$\psi_{\uparrow}(k) = \begin{pmatrix} s_{\uparrow}(k) \\ p_{x+iy\uparrow}(k) \end{pmatrix} \quad \psi_{\downarrow}(k) = \begin{pmatrix} s_{\downarrow}(k) \\ p_{x-iy\downarrow}(k) \end{pmatrix}$$

C. X. Liu et al, PRL 100, 2336601 (2008), R. R. Du's group, PRL 115 136804 (2015) .

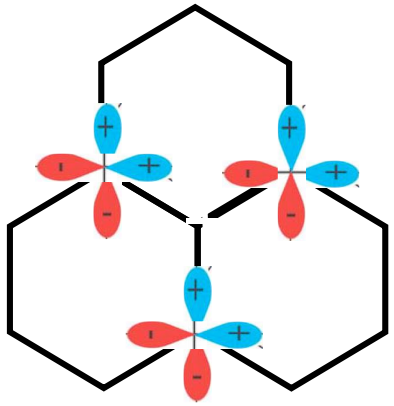
- InAs/GaSb type II quantum well

s and *p* spatially separated, inversion controlled by gate potential.

Topo-gap boosting mechanism

Gap at the atomic SO coupling (1eV)

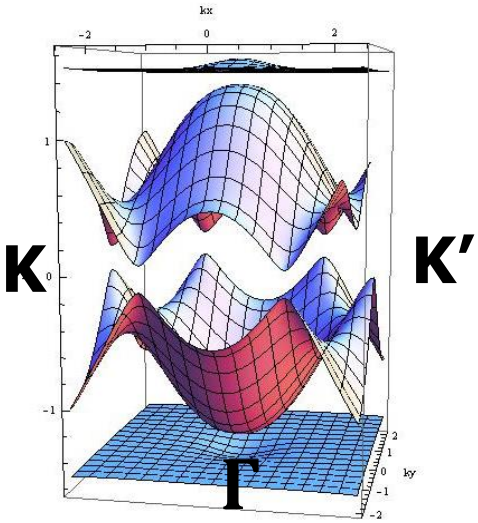
Orbital-active honeycomb systems



C. Wu, PRL 101, 186807 (2008)
M. Zhang, H. Hung, C. W. Zhang, C. Wu, PRA 83, 023615 (2011)
G. F. Zhang, Y. Li, C. Wu, PRB 90, 075114 (2014).

Real materials → Bismuthene on SiC

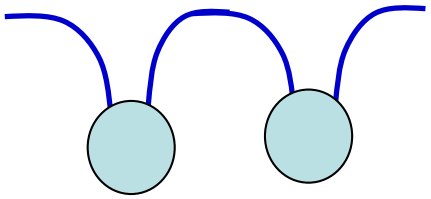
F. Reis, G. Li, L. Dudy, M. Bauernfeind, S. Glass, W. Hanke, R. Thomale, J. Schafer, and R. Claessen, Science (2017).
G. Li, W. Hanke, E. M. Hankiewicz, F. Reis, J. Schaefer, R. Claessen, C. Wu, R. Thomale, PRB 98, 165146 (2018).

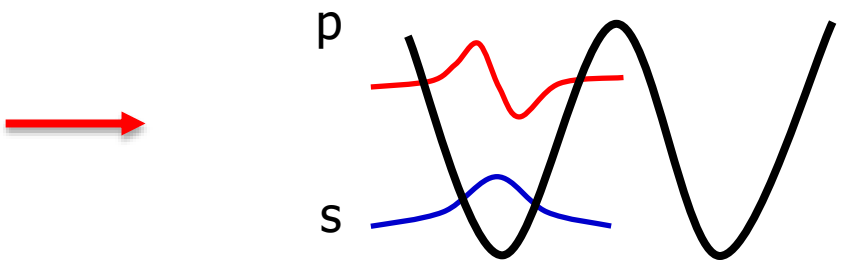


Stanene (Theory Xu, S. C. Zhang, Exp: Xue, Jia, He):

Topo-gap: solids v.s. AMO

- Solids: ionic core → soft pseudo-potential





(6s 6p no longer degenerate)

SO coupling: quantum spin Hall

$$\vec{\sigma}\cdot\vec{L} \rightarrow \sigma_x L_x + \sigma_y L_y + \sigma_z L_z$$

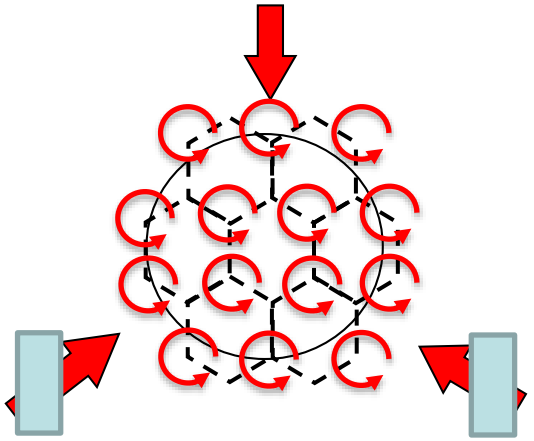
$$H_{SO} = -\lambda \sum_r \left(L_{\uparrow z}(\vec{r}) - L_{\downarrow z}(\vec{r})\right)$$

G. F. Zhang, Y. Li C. Wu, PRB 90 (2014).

- AMO: Rotate each site around its own center.

$$H_{zmn} = -\Omega \sum_r L_z(\vec{r})$$

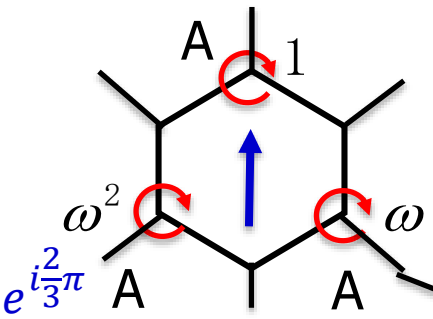
C. Wu, PRL 101, 186107 (2008); M. Zhang, Hung, C. Zhang, C. Wu, PRA (2011).



Topological gap = Atomic level spacing

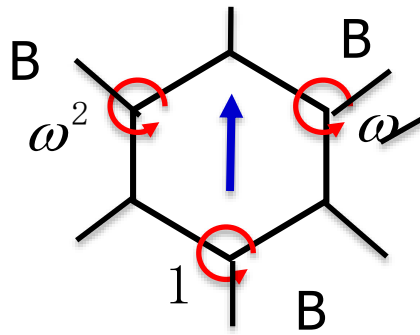
- A/B sublattices decouple due to *destructive interference*: non-bonding states at K (K′)

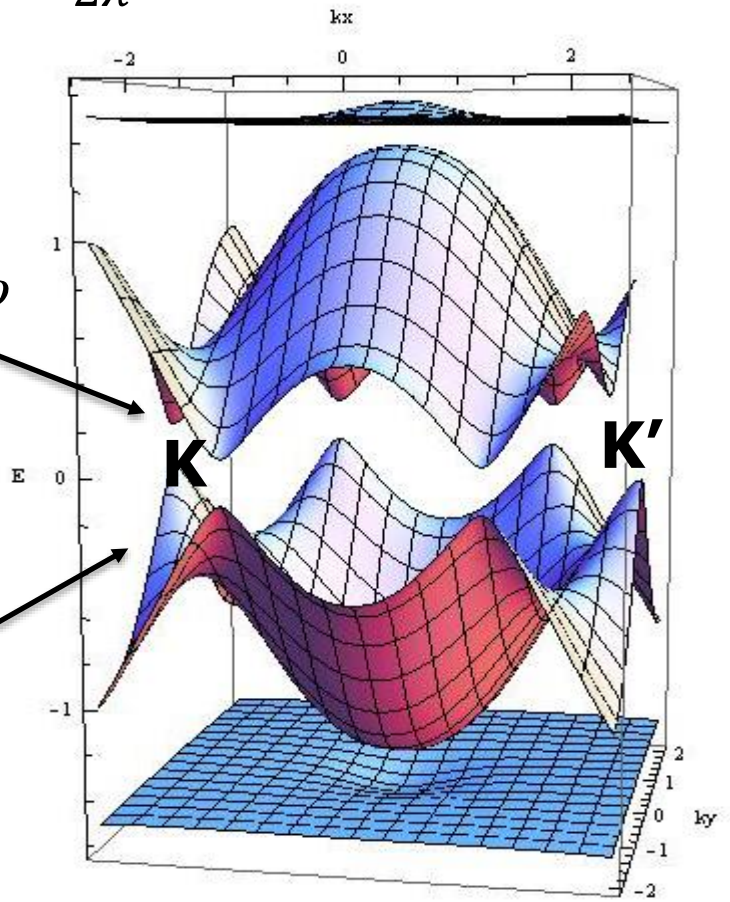
$$H_{SO} = \lambda L_z \sigma_z \rightarrow \Delta E = 2\lambda$$

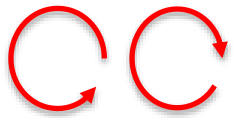


$\omega = e^{i\frac{2}{3}\pi}$

$\Delta E = 2\lambda$





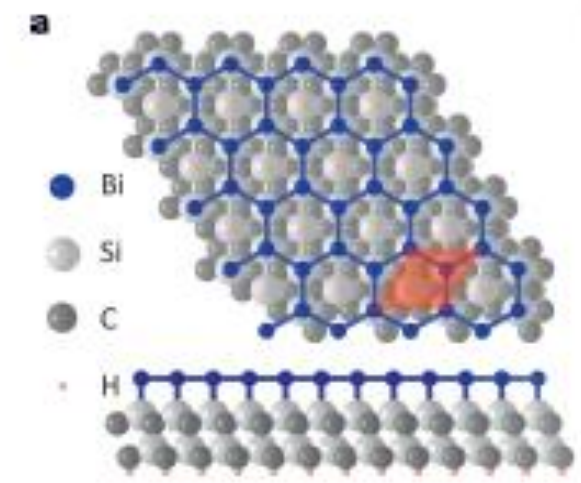


$p_x \pm ip_y$

G. F. Zhang, Y. Li, **CW**, PRB 90 (2014).

Bismuthene on the SiC substrate

- Monolayer – no buckling
- Large topo-gap ~0.67eV (STM)



weak s-p hybridization

p_z-orbital passivated by the SiC

p_x, p_y orbital-active honeycomb materials

Strong SO coupling

large topo-gap 2D materials

G. F. Zhang, Y. Li, C. Wu, PRB 90, 075114 (2014).
F. Reis, et al, Science 2017.
Gang Li, W. Hanke, Ewelina, M. Hankiewicz, J. Schafer, R. Claessen, C. Wu, and R. Thomale, PRB (2018).

Spectra of Bismuthene on SiC

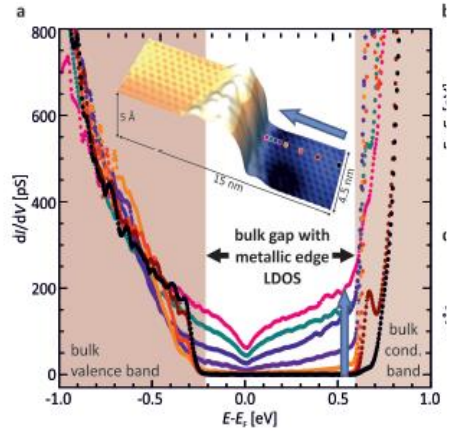
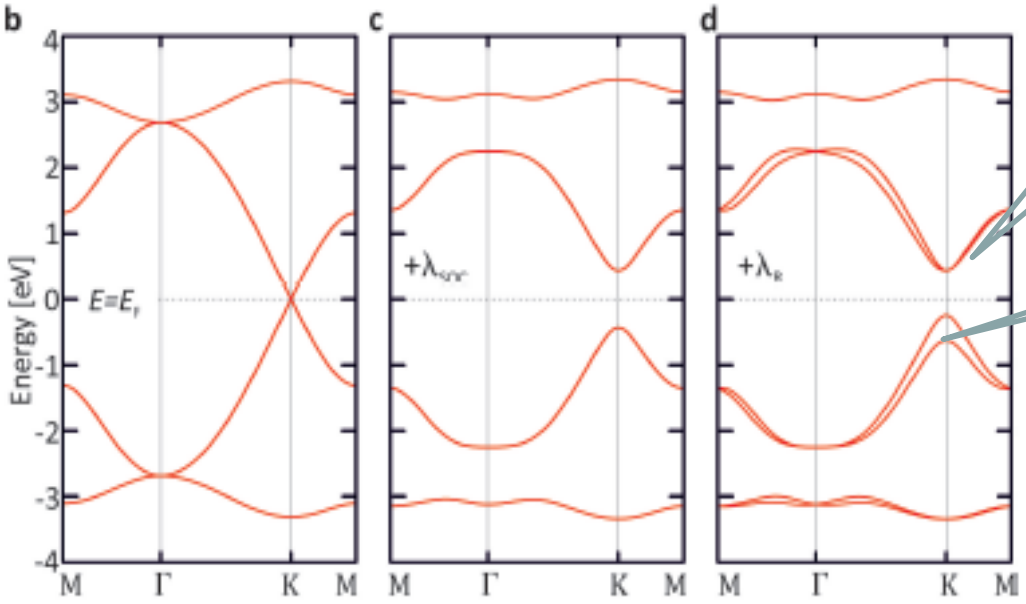


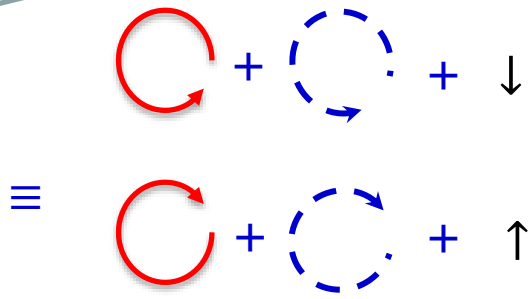
Figure 4 Spectroscopy of the Edge State

1. F. Reis, G. Li, et al Science (2017).
2. Gang Li, W. Hanke, Ewelina, M. Hankiewicz, J. Schafer, R. Claessen, C. Wu, and R. Thomale, PRB (2018).



$$j_z = \pm\frac{5}{2} \equiv \mp\frac{1}{2}$$

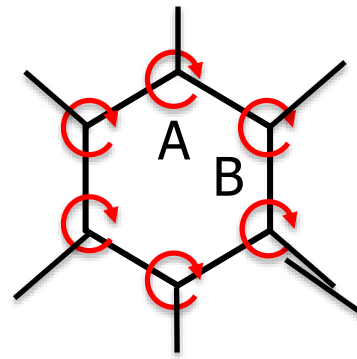
Double group:
Rashba splitting

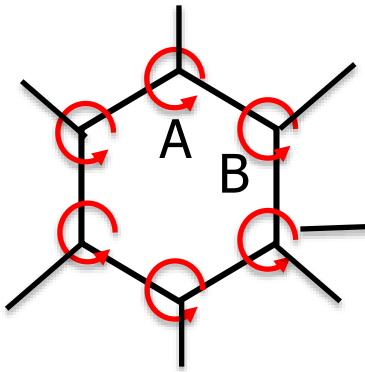


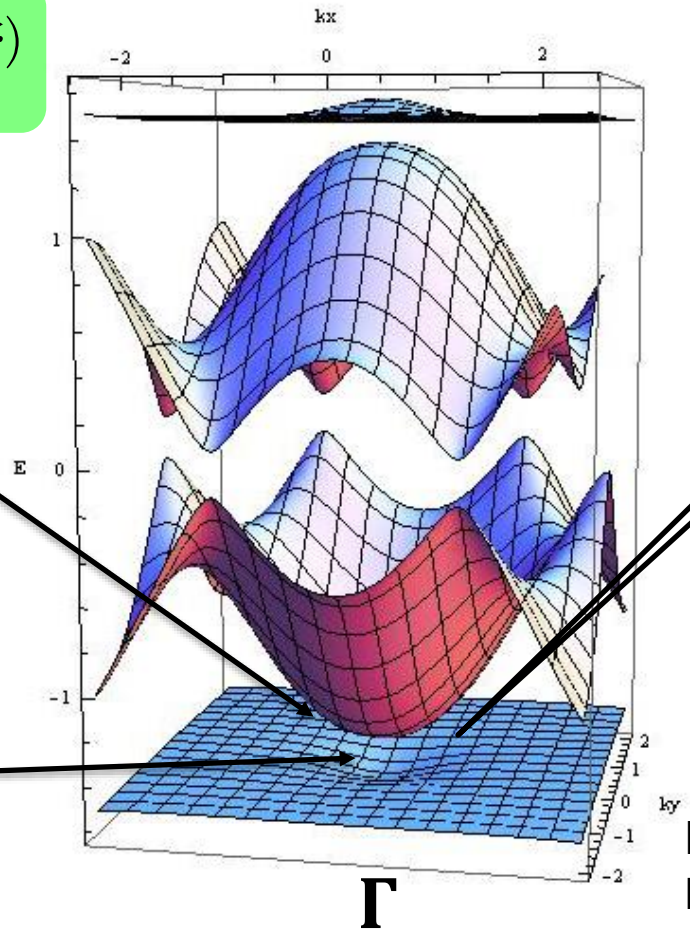
$$1 + 1 - \frac{1}{2} = \frac{3}{2} \equiv -\frac{3}{2}(mod\ 3)$$

Unification: Stanene - Γ -point

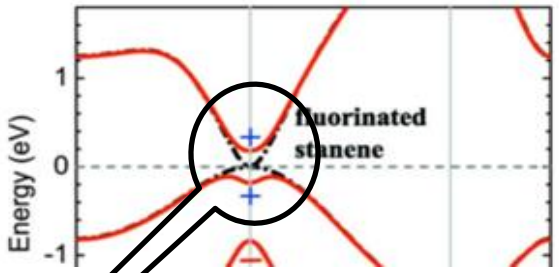
$$H_{SO,\uparrow} = -\lambda \sum_{r} L_z(\vec{r})$$







Γ



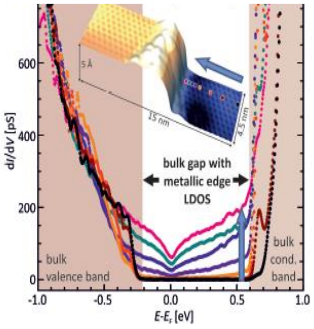
Y. Xu, et, al., PRL (2013)
S. Chen, et, al., PRB (2014)

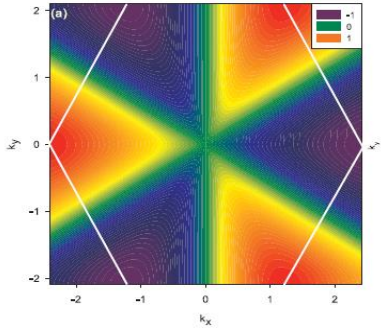
$$\Delta E = 2\lambda$$

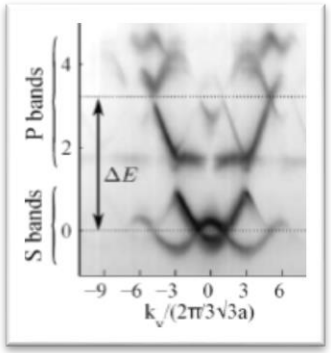
G. F. Zhang, Y. Li, C. Wu, PRB 90 (2014).

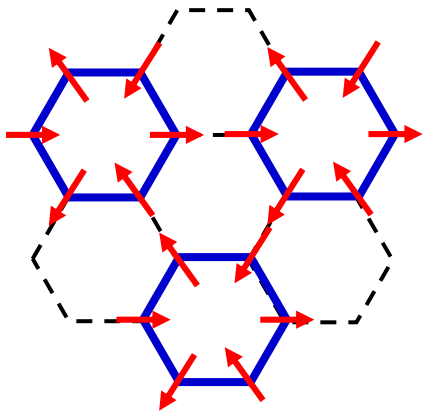
Experiments:
Menghan Liao, et al, arxiv1712.03695,
Yunyi Zang, et al, arXiv1711.07035
Fengfeng Zhang et al, Mature Materials 14, 1020 (2015).

large topo-gap at the atomic SO energy scale









Orbital-active honeycomb

$(p_x p_y)$, (d_{xz}, d_{yz})

$(d_{r^2-z^2}, d_{x^2-y^2})$

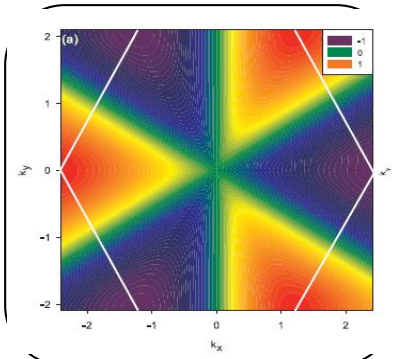
- Bismuthene, Stanene
- Polariton lattice
- Twisted bilayer graphene
- transition metal oxides

- FM , Wigner crystal in flat band
- Frustrated orbital exchange -120° model
- f-wave supercond.

band topology, orbital frustration

Lee, CW, Das Sarma, PRA (2010).

CW, PRL.100, 200406 (2008).

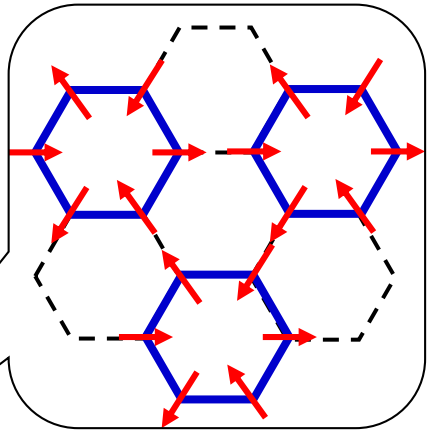


λ/t

QAHI(II)

semi-metal

QAHI(I)



120° model

U/t

f-wave SC

Mott Insulator

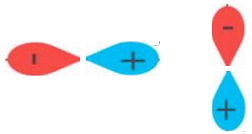
$NaNi_2BiO_6$

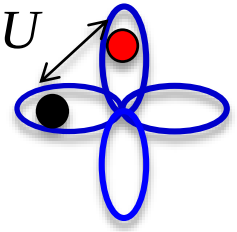
Doping (?)

arxiv1807.02528, Cava, Broholm et al.

Mott insulator of SPINLESS fermions: orbital exchange

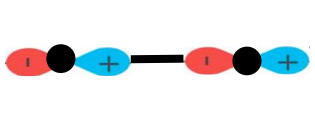
- Pseudo-spin representation.

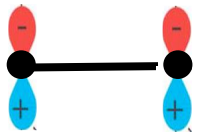




$$\tau_1 = \frac{1}{2}(p_x^+ p_x - p_y^+ p_y) \quad \tau_2 = \frac{1}{2}(p_x^+ p_y + p_y^+ p_x) \quad \tau_3 = \frac{i}{2}(p_x^+ p_y - p_y^+ p_x)$$

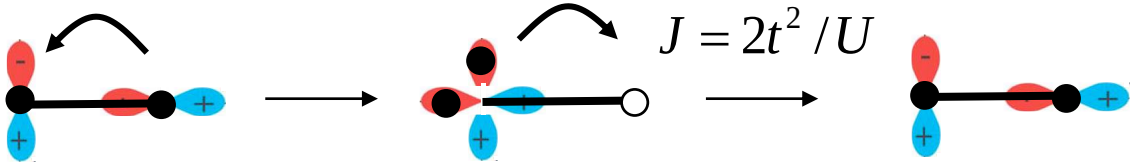
- Orbital exchange: no orbital flipping process.



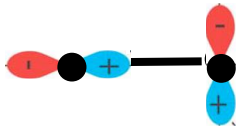


$J = 0$

$$H_{ex} = J\tau_1(r)\tau_1(r+\hat{x})$$



$J = 2t^2/U$

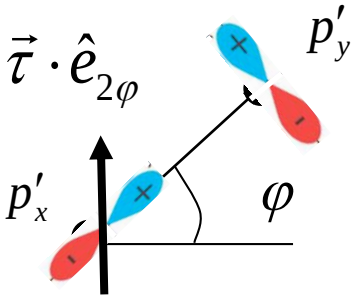


$J = 2t^2/U$

Hexagon lattice: quantum 120° model

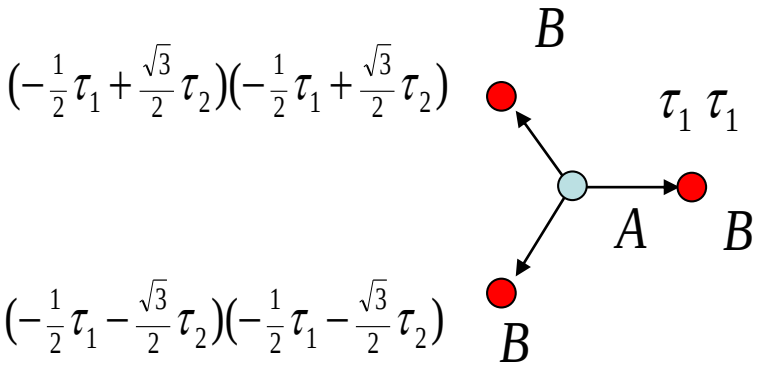
- Ising quantization axis depends on bond orientation.

p'_x, p'_y : eigen-states of $\vec{\tau}\cdot\hat{e}_{2\varphi} = \cos 2\varphi\,\tau_x + \sin 2\varphi\,\tau_y$



$$H_{ex} = J(\vec{\tau}(r)\cdot\hat{e}_{2\varphi})\,(\vec{\tau}(r+\hat{e}_{\varphi})\cdot\hat{e}_{2\varphi})$$

- Transformation: the Ising quantization axes → bond orientations.



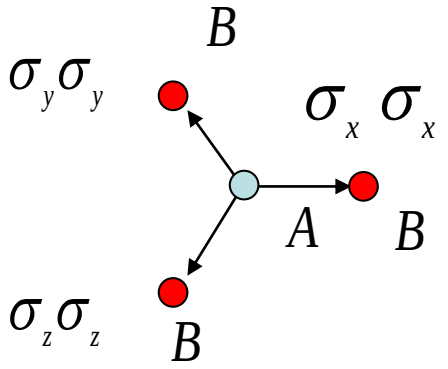
$$H_{ex} = -\sum_{r,r'} J(\vec{\tau}(r_i)\cdot\hat{e}_{ij})\,(\vec{\tau}(r'_j)\cdot\hat{e}_{ij})$$

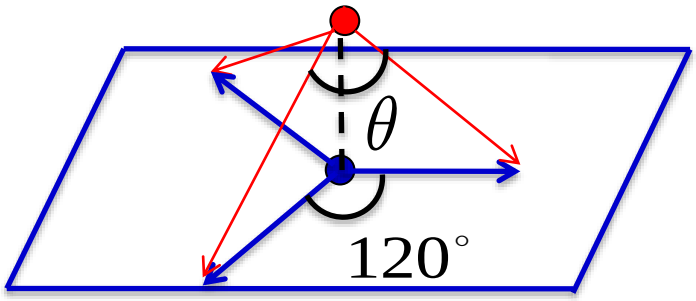
C. Wu et al, arxiv0701711v1; C. Wu, PRL 100, 200406 (2008). E. Zhao, and W. V. Liu, Phys. Rev. Lett. 100, 160403 (2008)

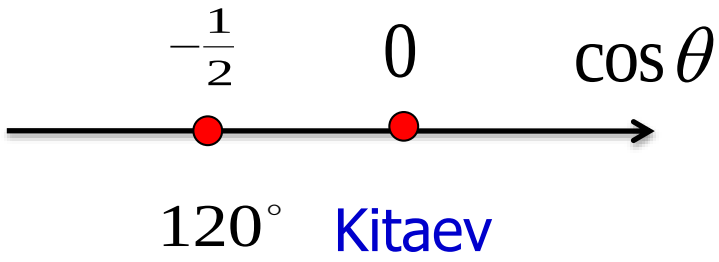
From the Kitaev model to 120 degree model

- cf. Kitaev model: Ising quantization axes form an orthogonal triad.

$$H_{kitaev} = -J \sum_{r \in A} (\sigma_x(r)\sigma_x(r+e_1) + \sigma_y(r)\sigma_y(r+e_2) + \sigma_z(r)\sigma_z(r+e_3))$$



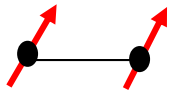




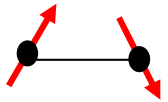
Large S picture: heavy-frustration of classic ground states

- Ground states: the two τ-vectors have the same projection along the bond orientation.

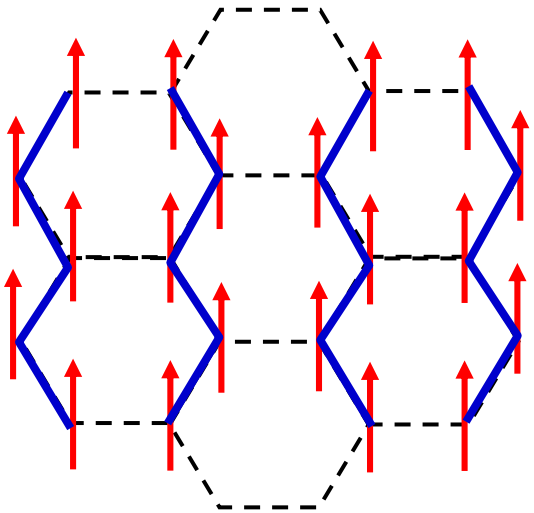
$$H_{ex} = \sum_{r,r'} J\{[(\vec{\tau}(r) - \vec{\tau}(r')] \cdot \hat{e}_{rr'}\}^2 + J\sum_{r} \tau_z^2(r)$$



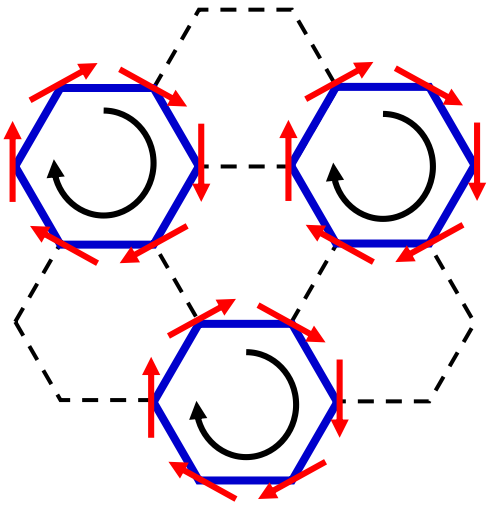
or



- Ferro-orbital configurations.

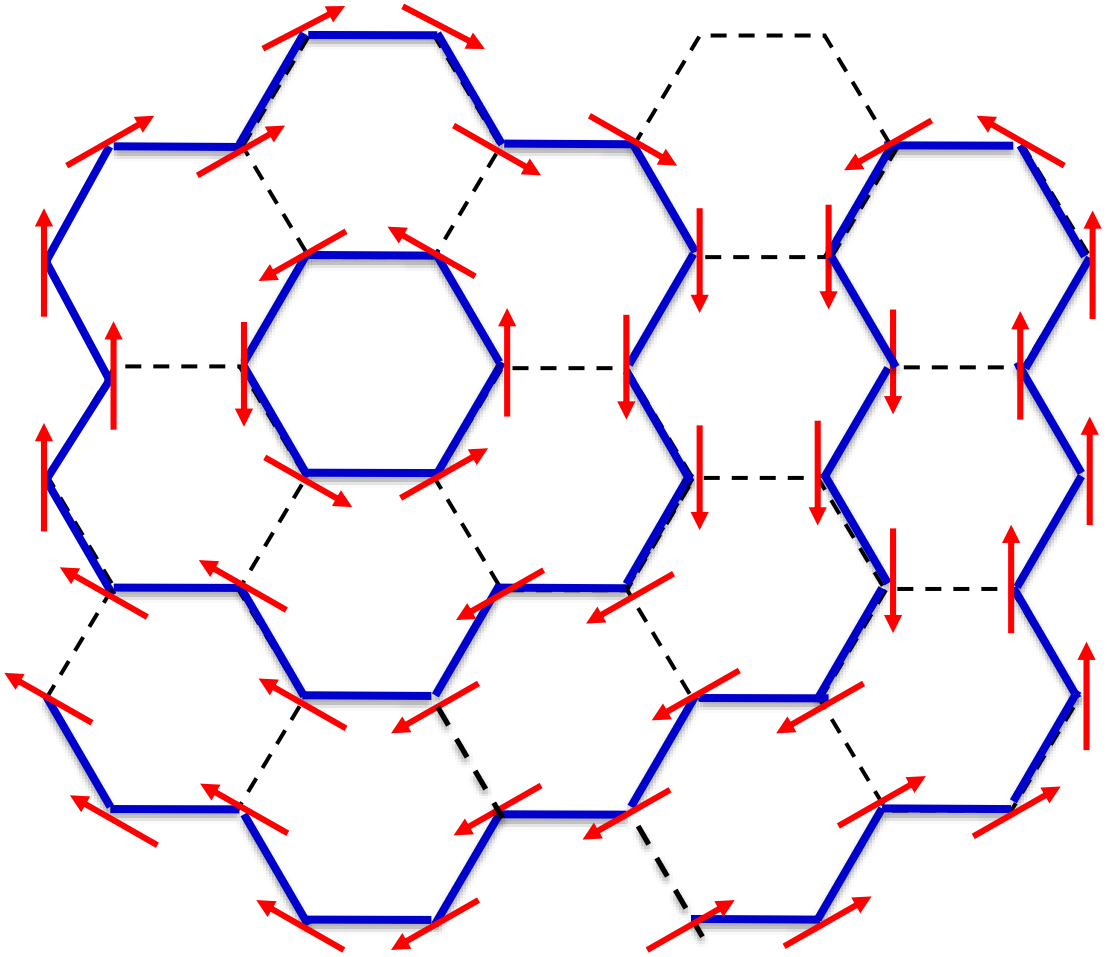


- Loop config: τ-vectors along the tangential directions.



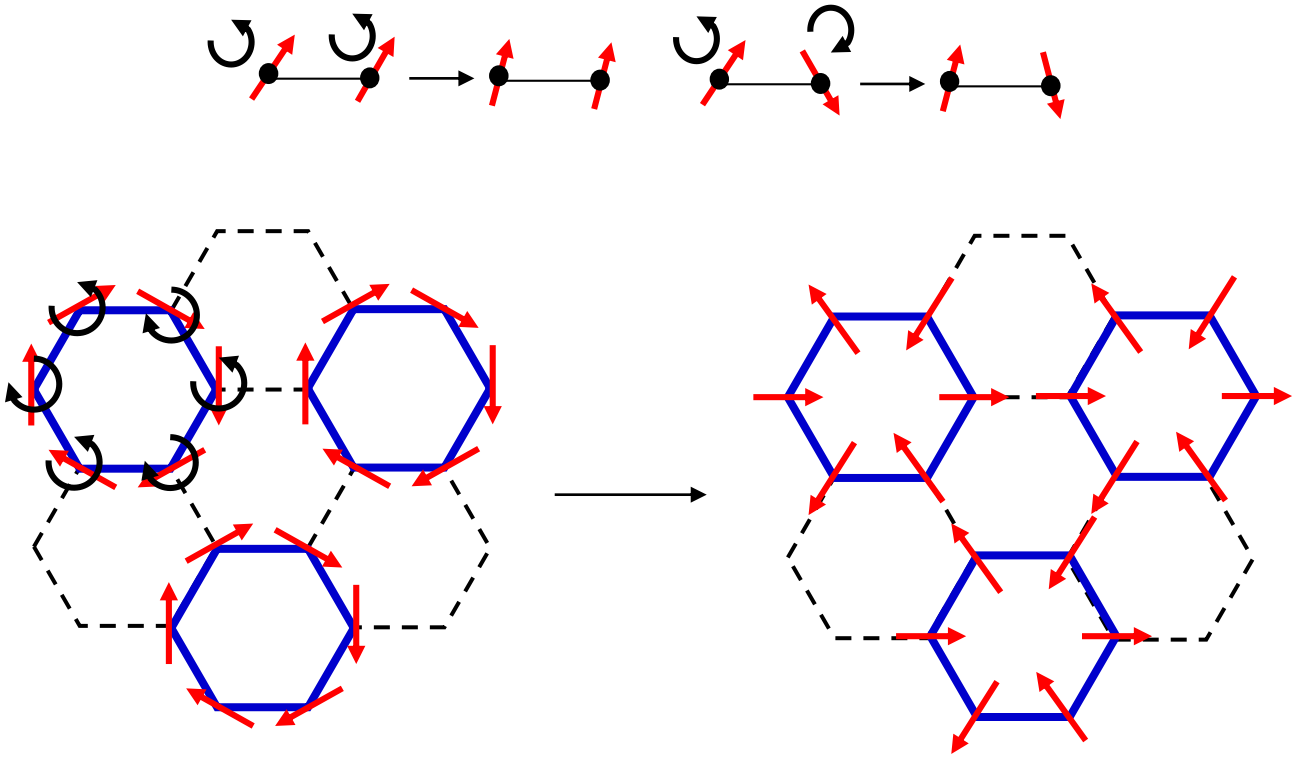
Heavy-degeneracy of the classic ground states

- General loop configurations

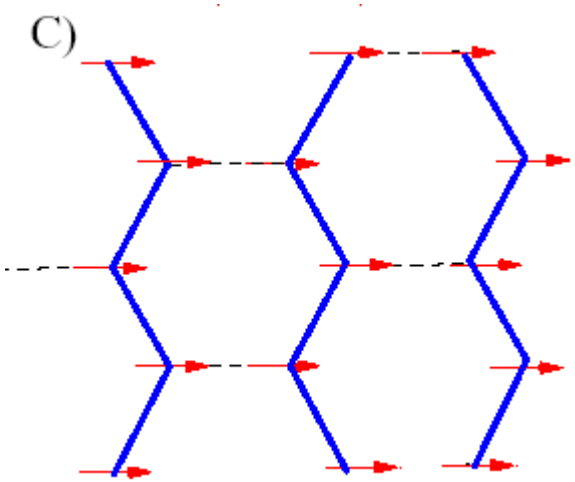


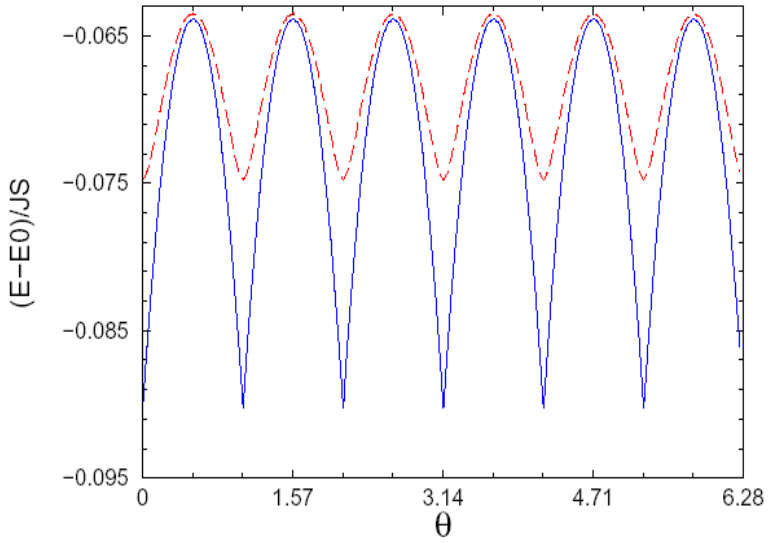
Global rotation degree of freedom

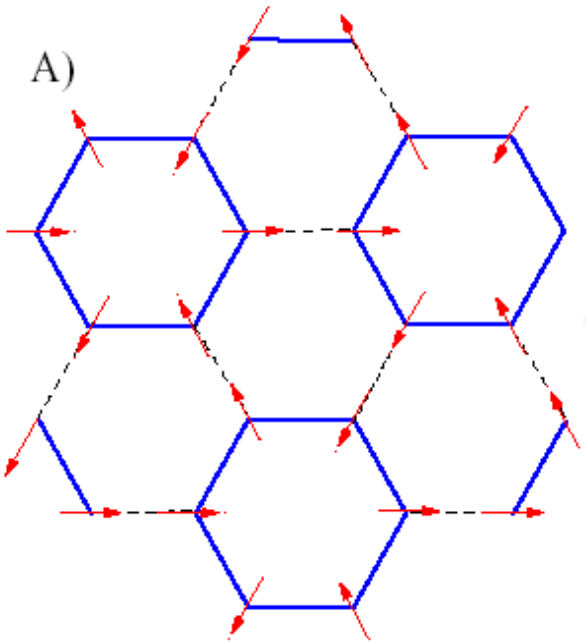
- Each loop config remains in the ground state manifold by a suitable arrangement of clockwise/anticlockwise rotation patterns.

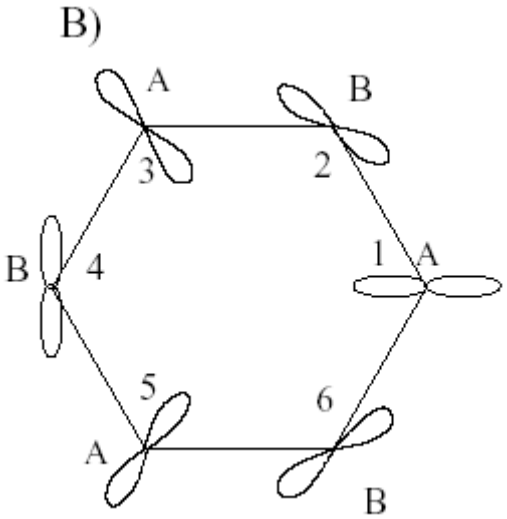


"Order from disorder": 1/S orbital-wave correction





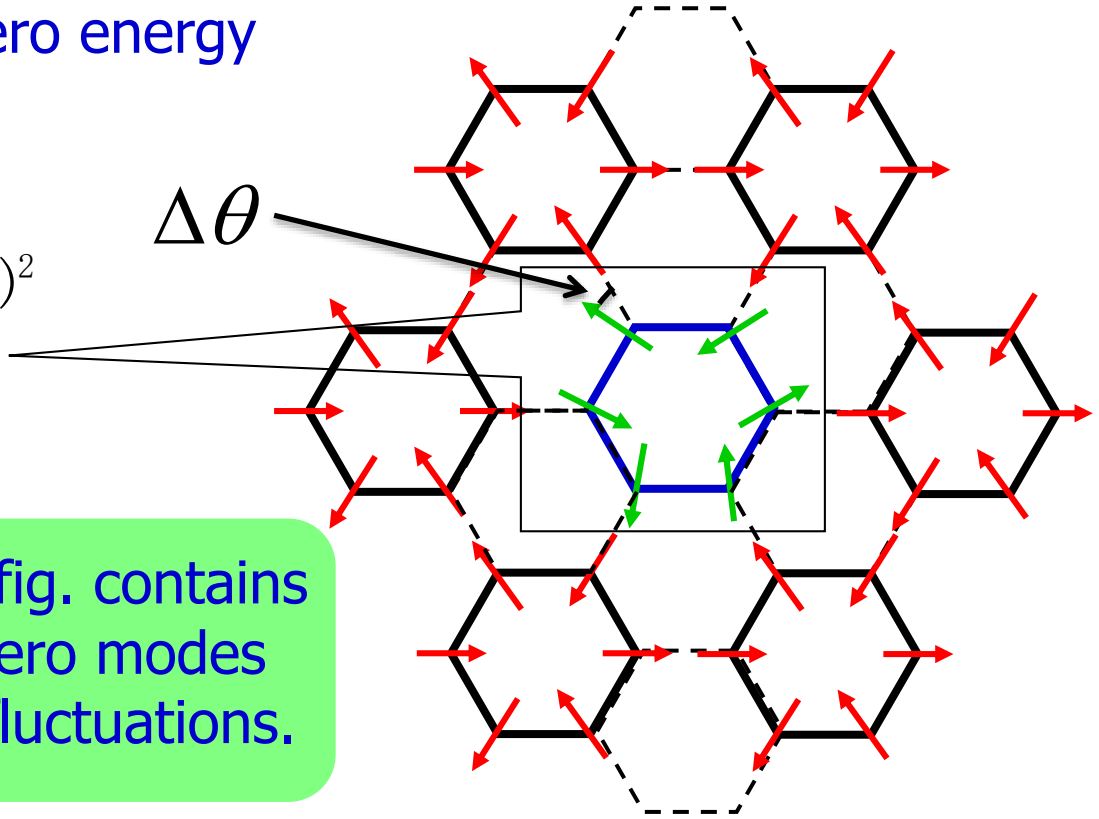




Zero energy orbital wave fluctuations

- Each loop has a local zero energy mode.

$$\Delta E = 6JS^2(1-\cos\Delta\theta)^2$$
$$\propto (\Delta\theta)^4$$

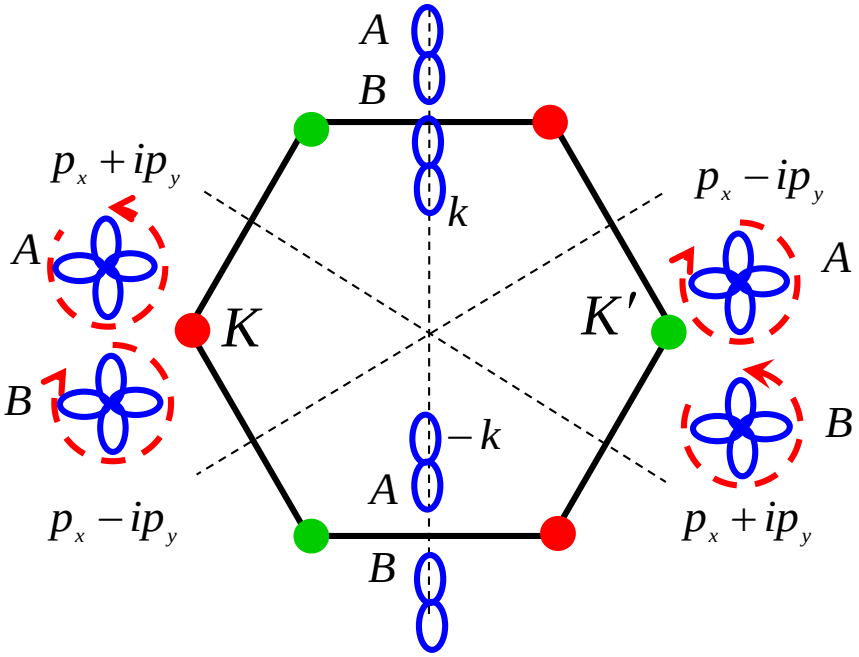


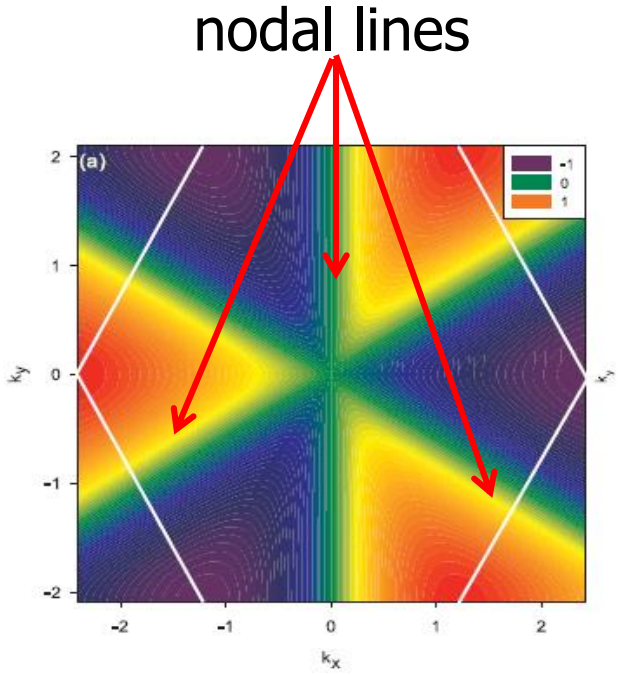
- The closest packed config. contains the maximal number of zero modes → selected by quantum fluctuations.

f-wave structure from conventional interaction

$$H_{\text{int}} = -U\sum_{\vec{r}} n_{p_x}(\vec{r})n_{p_y}(\vec{r}) = -U\sum_{\vec{r}} n_{p_x+ip_y}(\vec{r})n_{p_x-ip_y}(\vec{r})$$

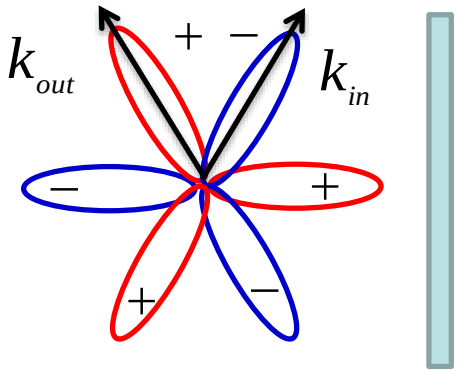
- Bisector lines are nodal lines: no interaction between TR pairs.
- The TR pair at K and K′ has the largest pairing.



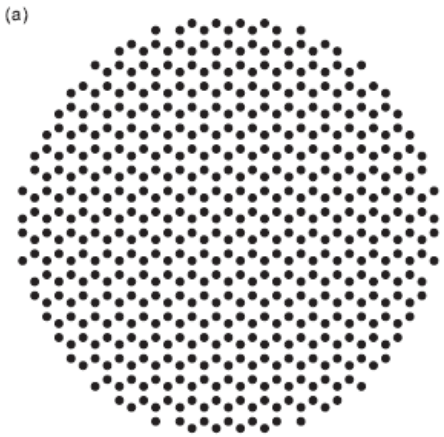


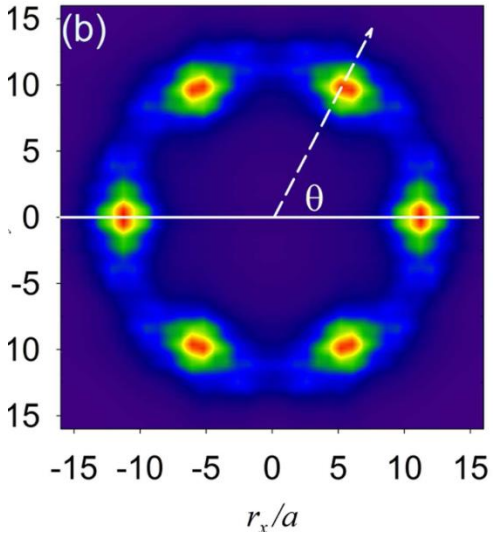
Orbital-assisted f-wave superconductivity

Zero energy Majorana boundary modes



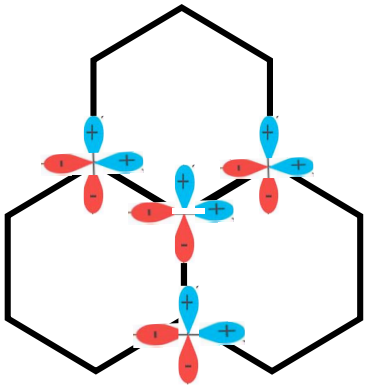
W. C. Lee, CW, S. Das Sarma, PRA 2010;

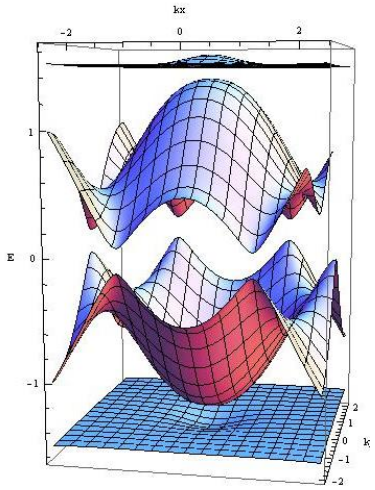


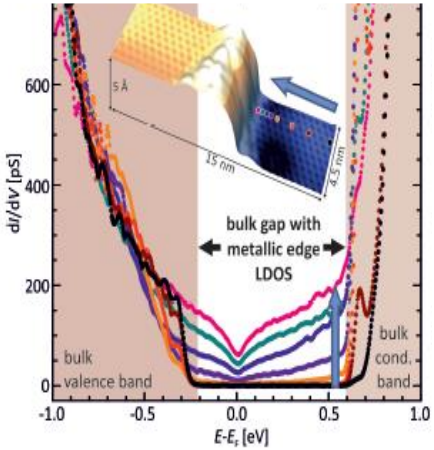


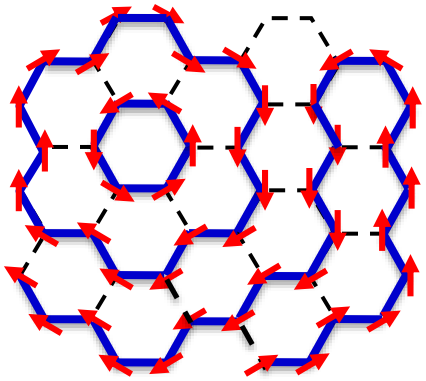
A unified framework for bismuthen, stanene, and more …

- p_x and p_y orbital-active honeycomb lattice
- Large topo gap to the scale of atomic spin-orbit coupling (1eV)
- Novel many-body physics: flat-band ferromagnetism, orbital frustration, f-wave superconductivity etc.



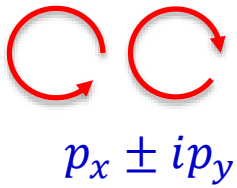




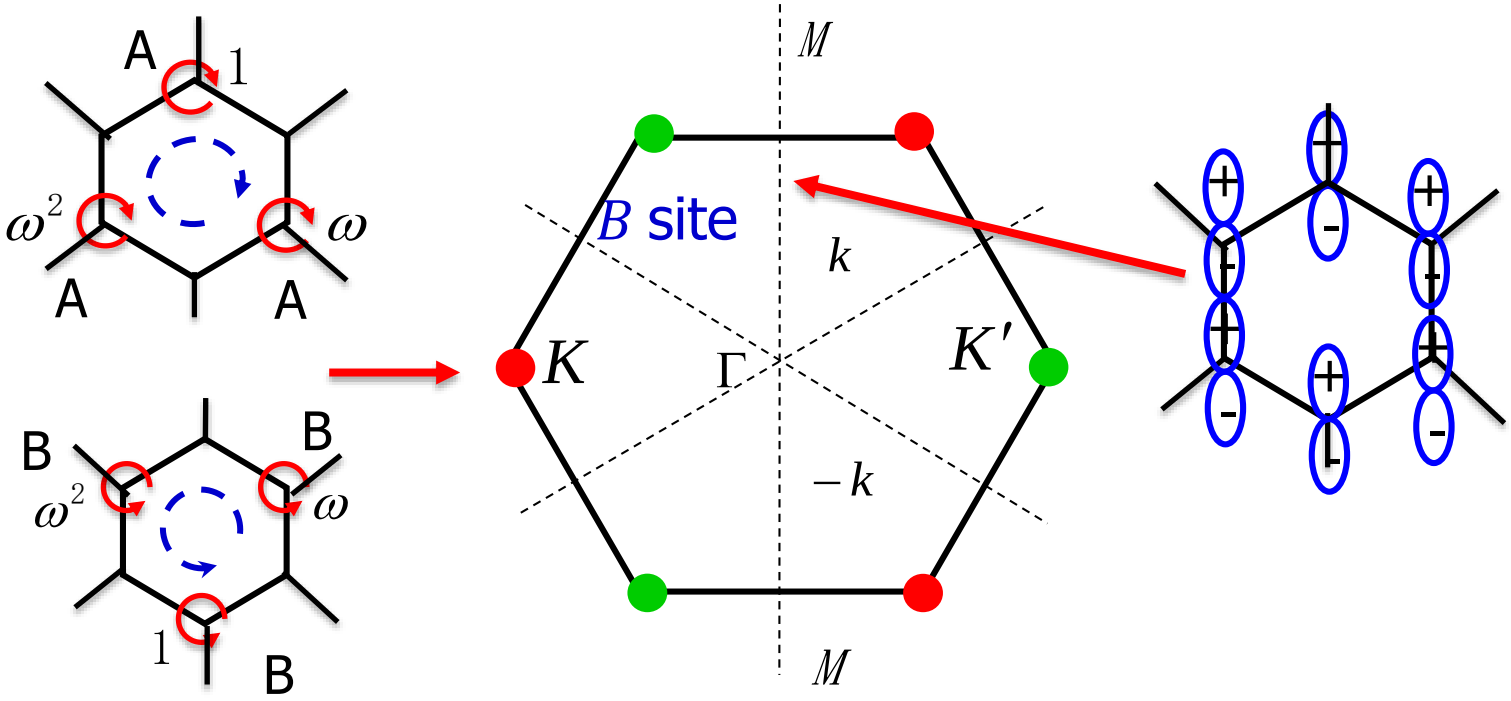


Back up!

Orbital configuration (Dirac band)



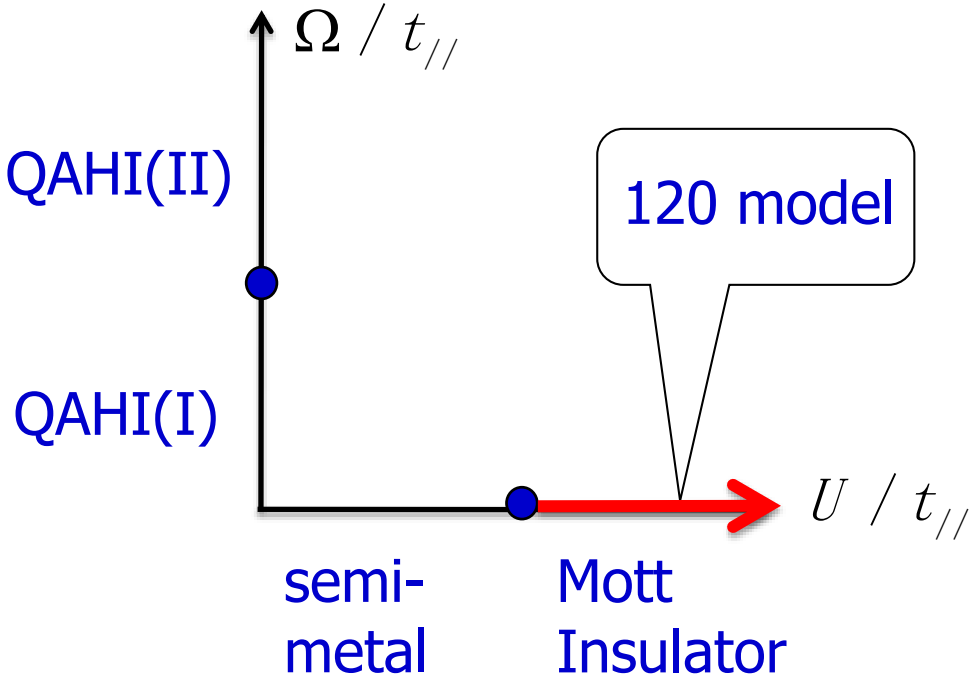
$p_x \pm ip_y$

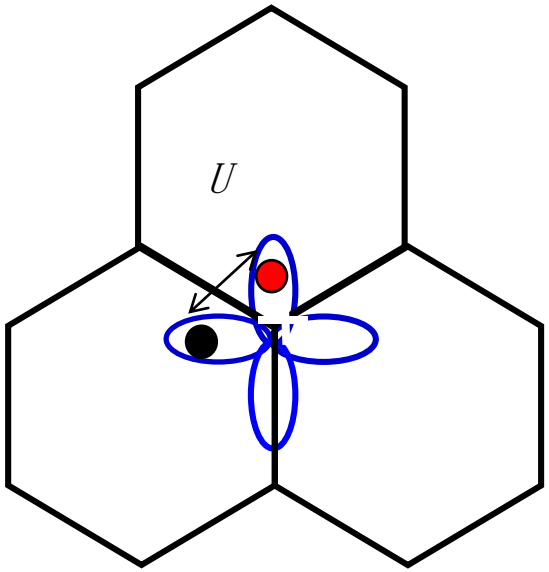


- **Real** eigen-orbitals along the M-Γ -M- line → f-wave pairing.
- **Complex** eigen-orbitals at K (K′) → large topo-gap with SO coupling.

C. Wu PRL 101, 2008; W. C. Lee, C. Wu, S. Das Sarma, PRA 2010;
G. F. Zhang, Y. Li C. Wu, PRB 90 (2014).

Add interactions (spinless fermions)





$$H_{\text{int}} = U \sum_{\vec{r}} n_{p_x}(\vec{r}) n_{p_y}(\vec{r})$$

$$H_0 = H_t - \Omega \sum_{r} L_z(\vec{r})$$

(Quantum) anomalous Hall state

- *k*-space Berry curvature.

$$\vec{A}(k) = \langle \psi_{L,k} \left| i\vec{\partial}_k \right| \psi_{L,k} \rangle, \qquad \Omega_z\left(\vec{k}\right) = \partial_{k_x} A_{k_y} - \partial_{k_y} A_{k_x}$$

- Anomalous velocity.

Luttinger, PR, 112 793 (1958),
Xiao, Chang, Niu, RMP 82, 1959 (2010).

$$\dot{\vec{r}} = \nabla_k \epsilon\left(\vec{k}\right) - \dot{\vec{k}} \times \vec{\Omega}(\vec{k})$$

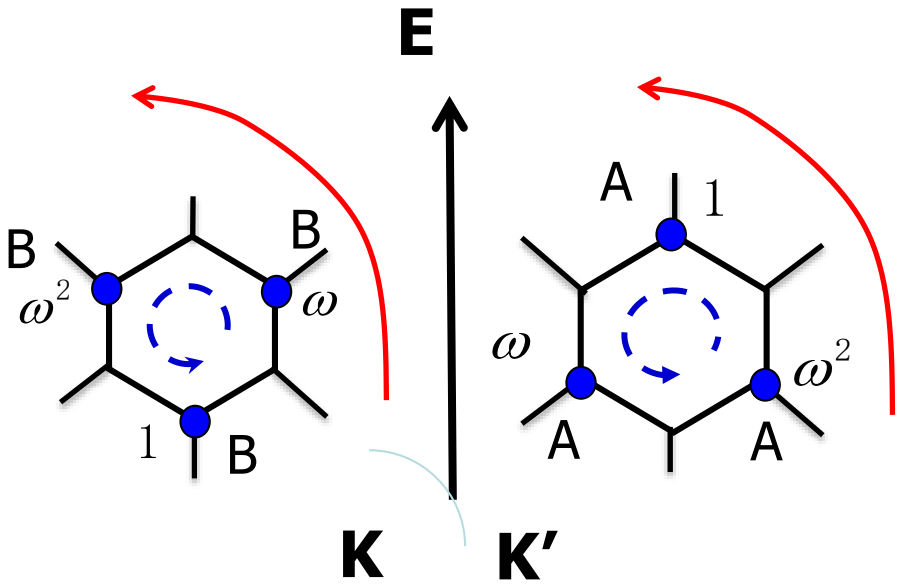
$$\dot{\vec{k}} = q\vec{E} + q\dot{\vec{r}} \times \vec{B}\,(\vec{r})$$

- Van Vleck (inter-band) response.

$$\sigma_{xy} = \frac{e^2}{h} \iint \frac{d^2\vec{k}}{2\pi} \Omega_z$$

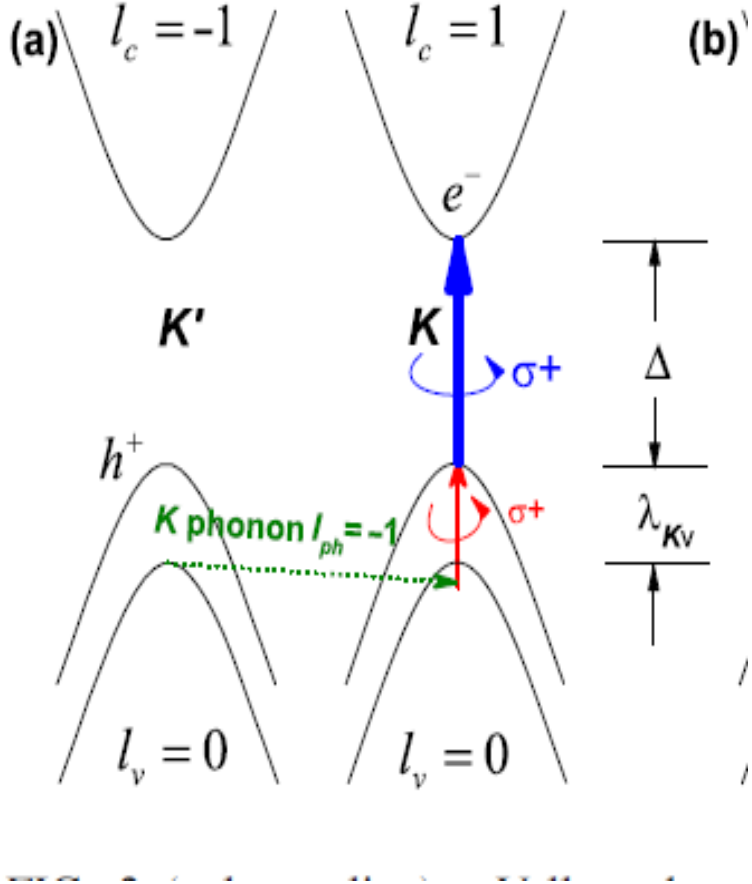
$$= \frac{e^2}{h} \iint \frac{d^2\vec{k}}{2\pi} \nabla \times \vec{A}\left(\vec{k}\right) = \pm \frac{e^2}{h}$$

$$\boldsymbol{\Omega_z(K) = \Omega_z(K')}$$



Thouless, Kohmoto, Nightingale, den Nijis, PRL 49, 405 (1982)

Creation of chiral phonon and large momentum exciton



1. Right-handed light → exciton at K-valley

2. Another right-handed light → hole scattered to K'-valley by absorbing phonon and emitting a chiral phonon (K-K'=2K=K')

3. Electron and hole are in different valleys → large momentum exciton.

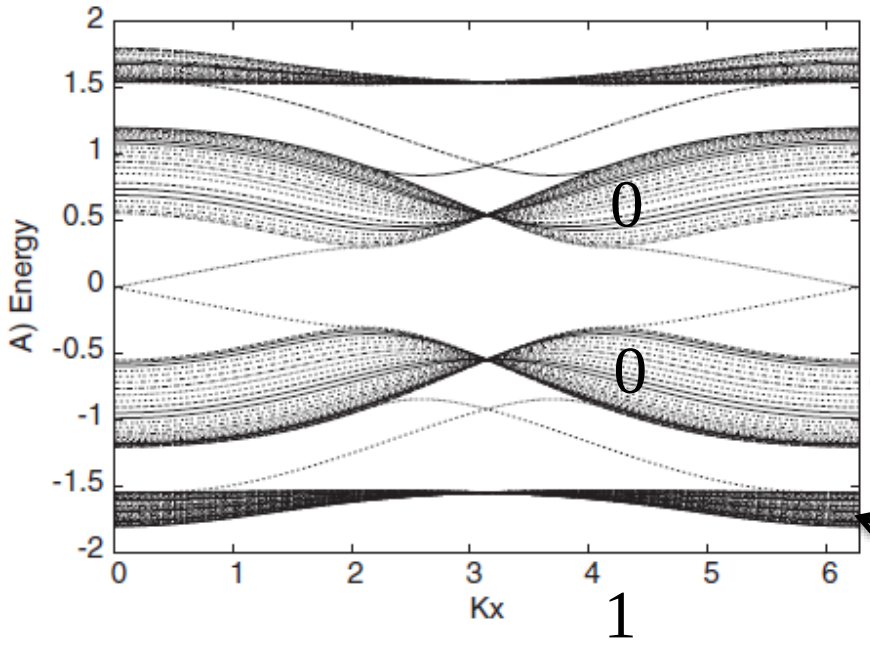
$$\Delta = 1.65\text{eV}$$

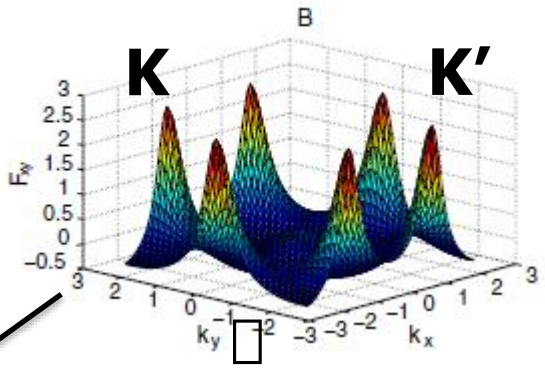
$$\lambda_{\text{Kv}} = 0.15eV$$

Edge spectra and Berry curvature (spin ↑)

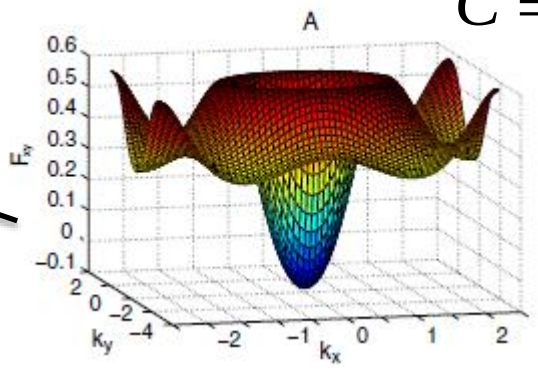
$C = 0 \approx 1 + (-1)$

$\lambda = 0.3t_{//}$ $C = -1$





$C = 1$

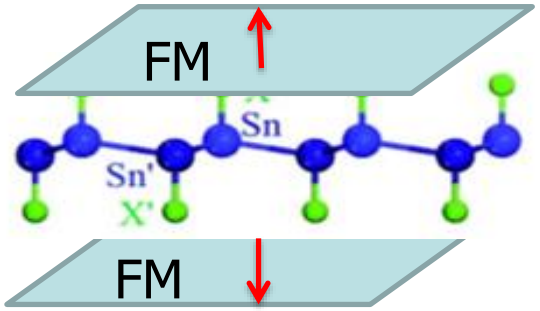


C. Wu, Phys. Rev. Lett. 101, 186807 (2008).

Quantum anomalous Hall (QAH): a triangle relation

- The 3rd gap mechanism: Neel exchange.

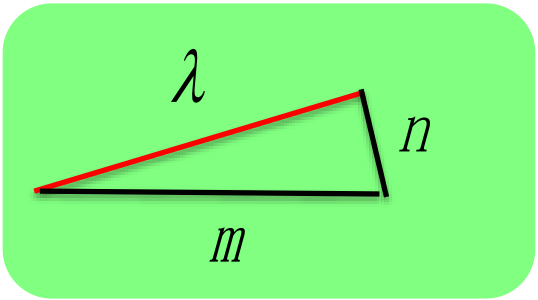
$$H_N = -n\sum_r (S_{zA}(r) - S_{z,B}(r))$$



- Superpose charge and spin sub-lattice asymmetry.

spin-up spin-down

$$m + n > \lambda > |m - n|$$



topo trivial topo non-trivial

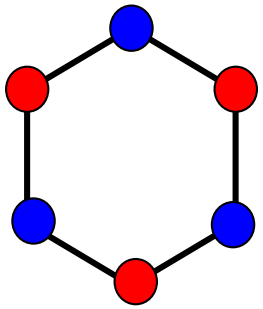
- QAH -- **Three players**: none should be too large, too small either.

G. F. Zhang, Y. Li, C. Wu, PRB 90 (2014).
Q.F. Liang, L.H. Wu, X. Hu, NJP 2013.

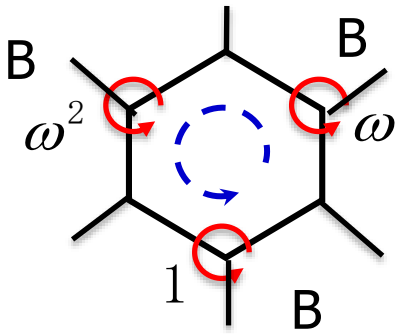
Gaps due to sub-lattice asymmetry $m > \ell$ (cf. MoS_2)

- Gaps around K (K') → valley Hall.

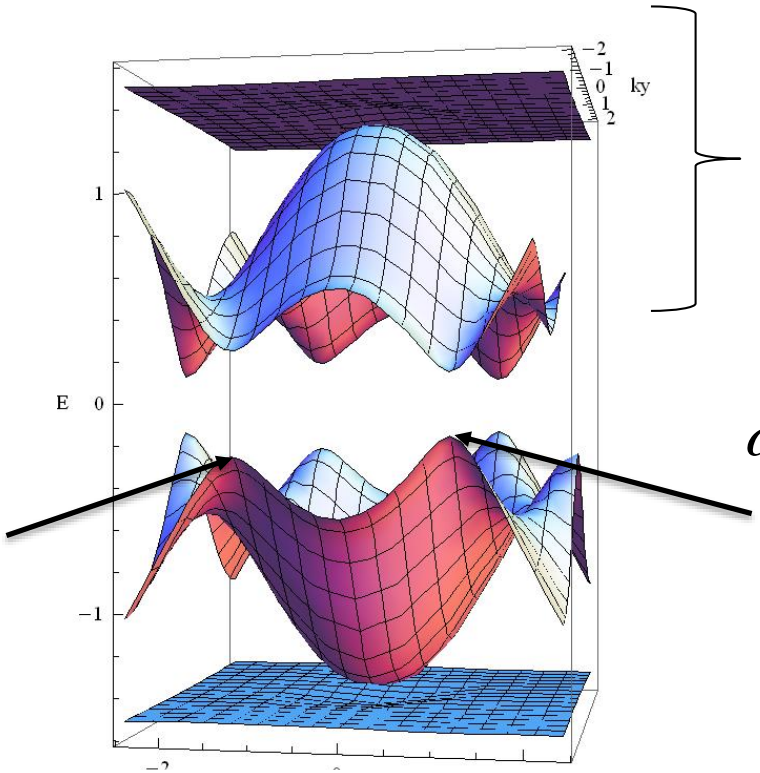
$$H_M = -m\sum_r (n_A(r) - n_B(r))$$



$d_{x^2-y^2 \pm 2ixy}$

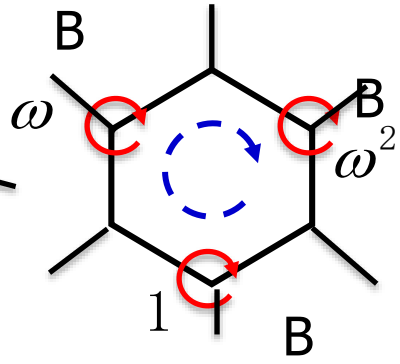


$\Delta E = -(m + \lambda)$



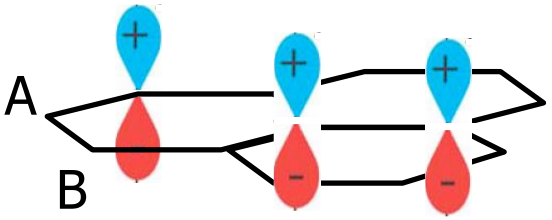
MoS_2: upper bands are replaced by

$d_{r^2-3z^2}$

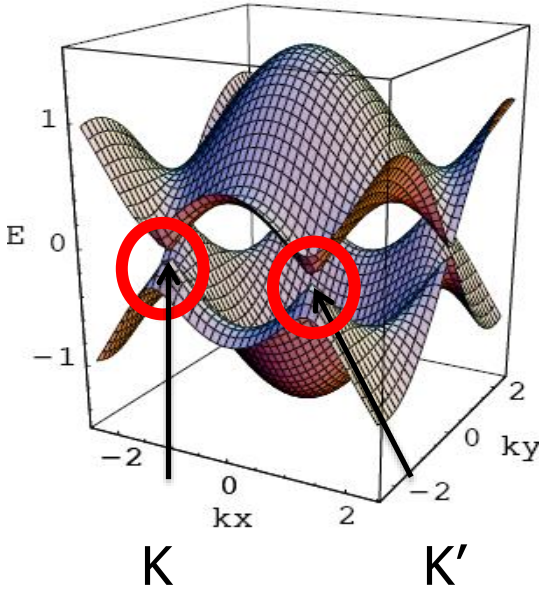


$\Delta E = -(m - \lambda)$

Honeycomb lattice system (graphene)



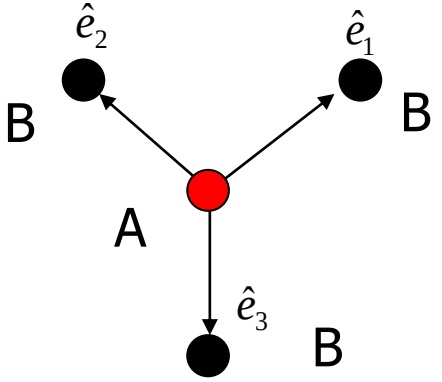
$$\psi(k) = \begin{pmatrix} c_A(k) \\ c_B(k) \end{pmatrix}$$



- 2-level in a planar pseudo-B field.

$$H\left(\vec{k}\right) = \vec{h}\left(\vec{k}\right) \cdot \vec{\tau}$$

$$h_x\left(\vec{k}\right) + i h_y\left(\vec{k}\right) = \sum_{i=1}^{3} e^{i\vec{k}\cdot\hat{e}_i}, \qquad h_z\left(\vec{k}\right) = 0$$



- Symmetry and topology protection:

  gapless Dirac cones ←→ $\vec{h}(K) = \vec{h}(K') = 0$.

Selected References
1. G. Li, W. Hanke, E. M. Hankiewicz, F. Reis, J. Schaefer, R. Claessen, C. Wu , R. Thomale, PRB 98, 165146 (2018).
2. G. F. Zhang, Yi Li, C. Wu, PRB 90, 075114 (2014).
3. M. Zhang, H. Hung, C.W. Zhang, C. Wu, PRA 83, 023615 (2011).
4. C. Wu, PRL 101, 186807 (2008).
5. C. Wu, PRL 100, 200406 (2008).
6. C. Wu, D. Bergman, L. Balents, and S. Das Sarma, PRL. 99, 70401 (2007).

Early work: on-line video

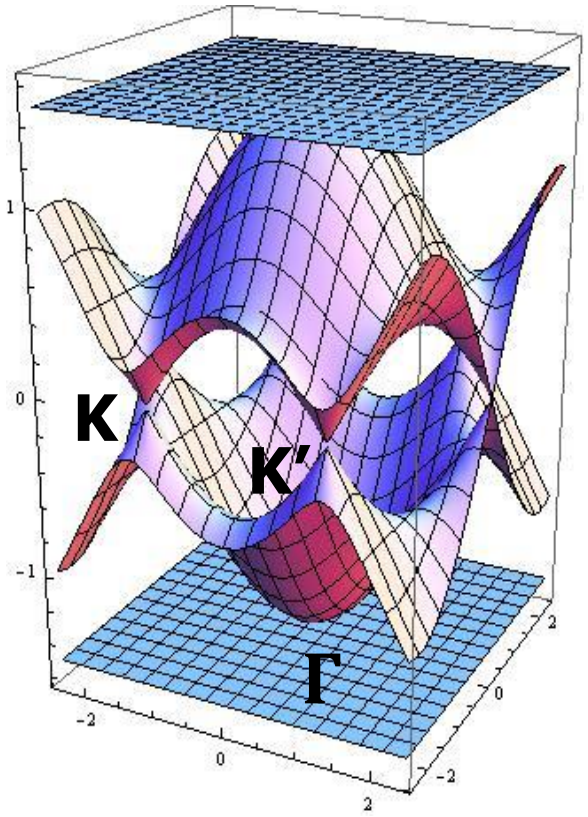
http://online.kitp.ucsb.edu/online/lowdim_c09/wu/

My research webpage

https://wucj.physics.ucsd.edu/research/topo/pQSH.html

https://wucj.physics.ucsd.edu/research/coldatom/pband.html

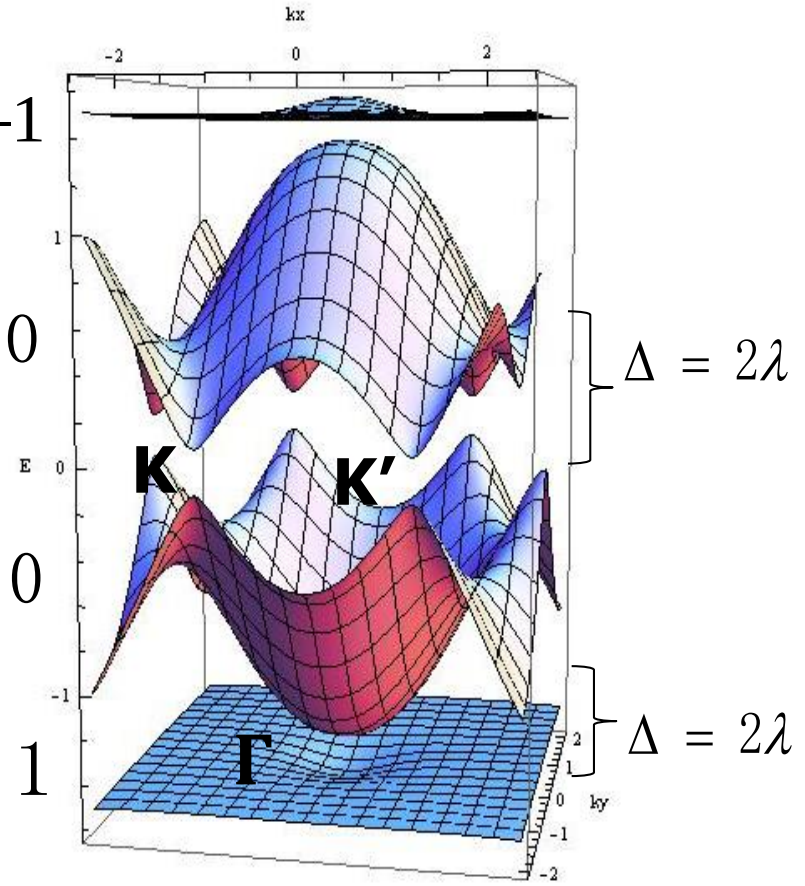
Large topo-gaps ~ atomic SO coupling strength



$$H_{so\uparrow} = -\lambda \sum_r L_z(\vec{r})$$

$$H_{\Omega} = -\Omega \sum_r L_z(\vec{r})$$

$C = -1$



Little group:	Ω =0	Ω>0	degeneracy
Γ	D_6	C_6	2→1+1
K(K′)	D_3	C_3	2→1+1