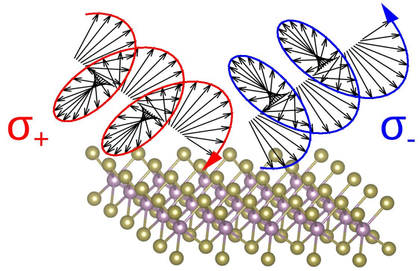
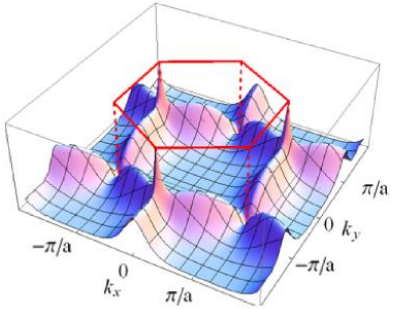
Valley and pseudospin polarization in two-dimensional hexagonal lattice



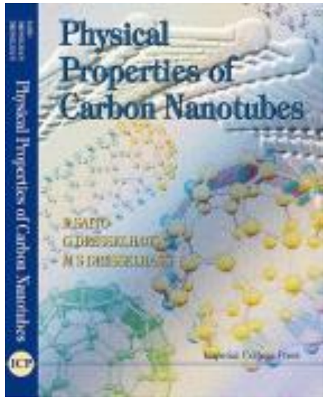
Riichiro Saito

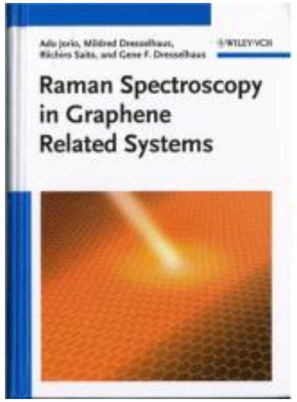


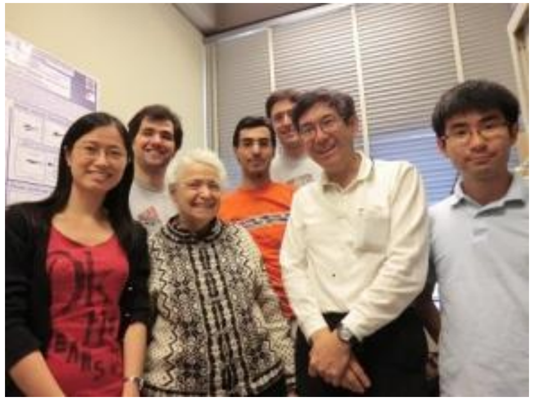
Yuki Tatsumi

Kazu Gharamkari

Department of Physics, Graduate School of Science,
Tohoku University, Sendai, Japan

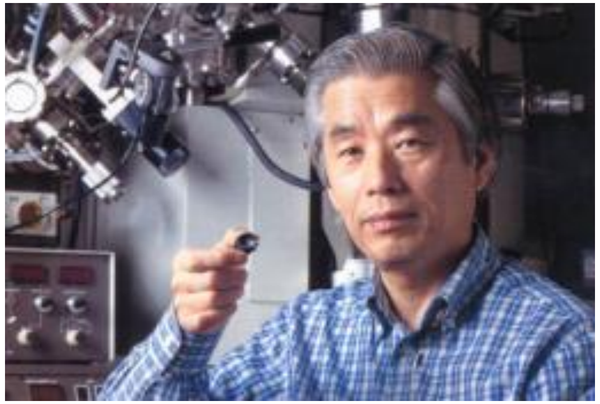




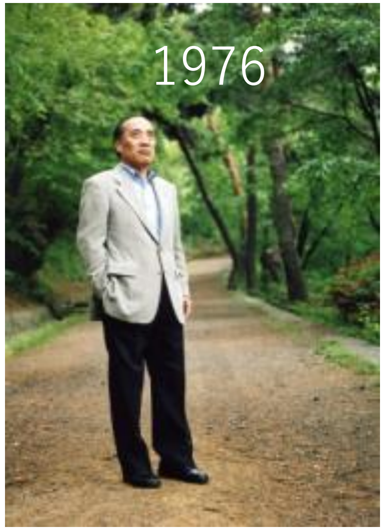


30 years of Nano Carbon
Fullerene-Nanotube-Graphene

2004

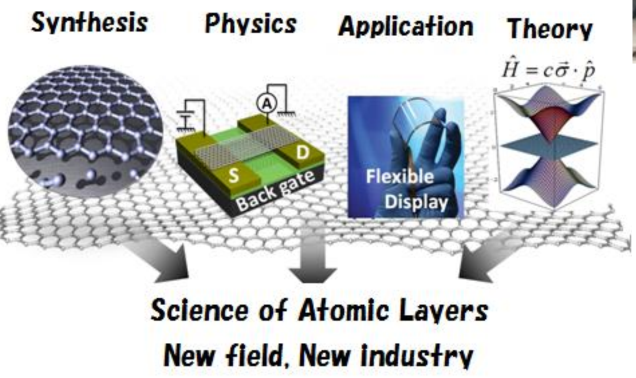


1991



JAPAN MEXT grant “Science of Atomic Layers”

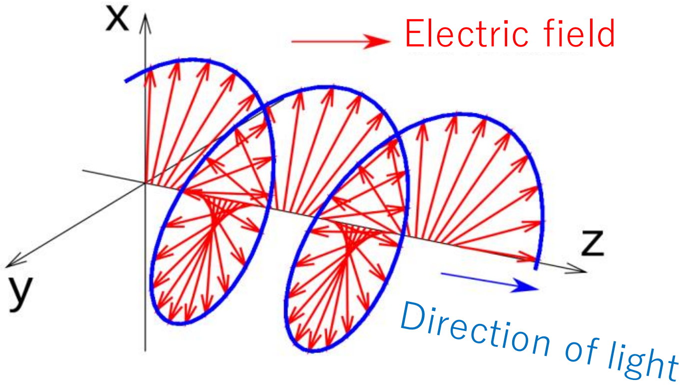
http://flex.phys.tohoku.ac.jp/satl 2013.4 - 2018.3

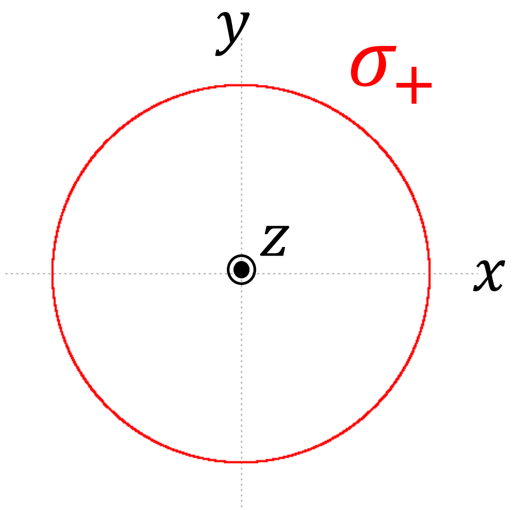


- **896 published papers from SATL, Japan !!**
- **Supply 2D samples (h-BN, graphene, TMD)**
- **Continue Collaborations with you !!**

"Spin" Angular momentum of circularly polarized light

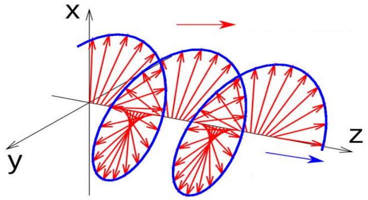
	Left-handed (σ_+)	Right-handed (σ_-)	Linear
Polarization the Jones vector	$P_+ \propto \begin{pmatrix} 1 \\ e^{+\frac{\pi}{2}i} \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}$	$P_- \propto \begin{pmatrix} 1 \\ e^{-\frac{\pi}{2}i} \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}$	$P = \begin{pmatrix} a \\ b \\ 0 \end{pmatrix}$ $a, b \in \mathbb{R}$
Helicity σ ("spin" angular momentum)	$+\hbar$	$-\hbar$	0





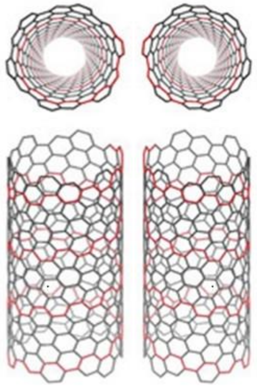
$$P_+ = \underbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}_{\vec{x}} + i \underbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}_{\vec{y}} = \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}$$

Circular polarized light
→Linear combination of $\vec{x}$ and $\vec{y}$



Left-handed (σ_+)
Right-handed (σ_-)

Optical phenomena by circularly polarized light
- *Optical absorption is different*! –

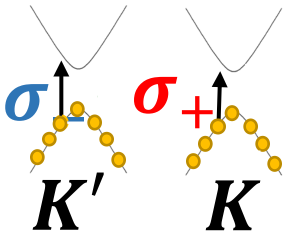


1. Circhular Dichroism (CD):

Different absorption for σ_+ and σ_-
Left and right handed molecule (or CNT)

N. Sato et al., *Phys. Rev. B*. **95**, 155436 (2017)

$$\tan\theta = \frac{I(\sigma_+) - I(\sigma_-)}{I(\sigma_+) + I(\sigma_-)}$$

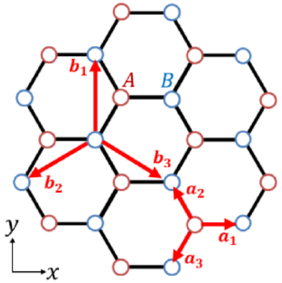


2. Valley Polarization (VP)

Different absorption at K and K’
Different sign of Berry curvature at K and K’
X. Xu et al. *Nat. Phys.* **10** 343 (2014)
K. Ghalamkari et al, *J. Phys. Soc. Jpn.*, **87**, 063708 (2018)

$$\tan V = \frac{I_\sigma(K) - I_\sigma(K')}{I_\sigma(K) + I_\sigma(K')}$$

$(\sigma = \sigma_+, \sigma_-)$



3. Pseudo-spin Polarization (PP)

Wavefunction coefficients for A and B atoms
inversion of conduction and valence bands

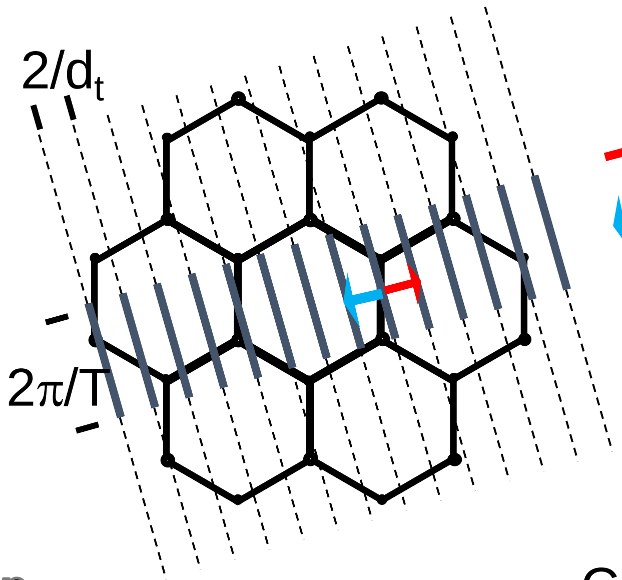
K. Sasaki and RS, *Prog. Theor. Phys. Suppl*. **176**, 253, (2008).

$$\tan p = \frac{|C_A^d|^2 - |C_B^d|^2}{|C_A^d|^2 + |C_B^d|^2}$$

$(d = v, c)$

CD: circular dichroism of CNT

N. Sato, Y. Tatsumi, RS, *Phys. Rev. B.* **95**, 155436 (2017)

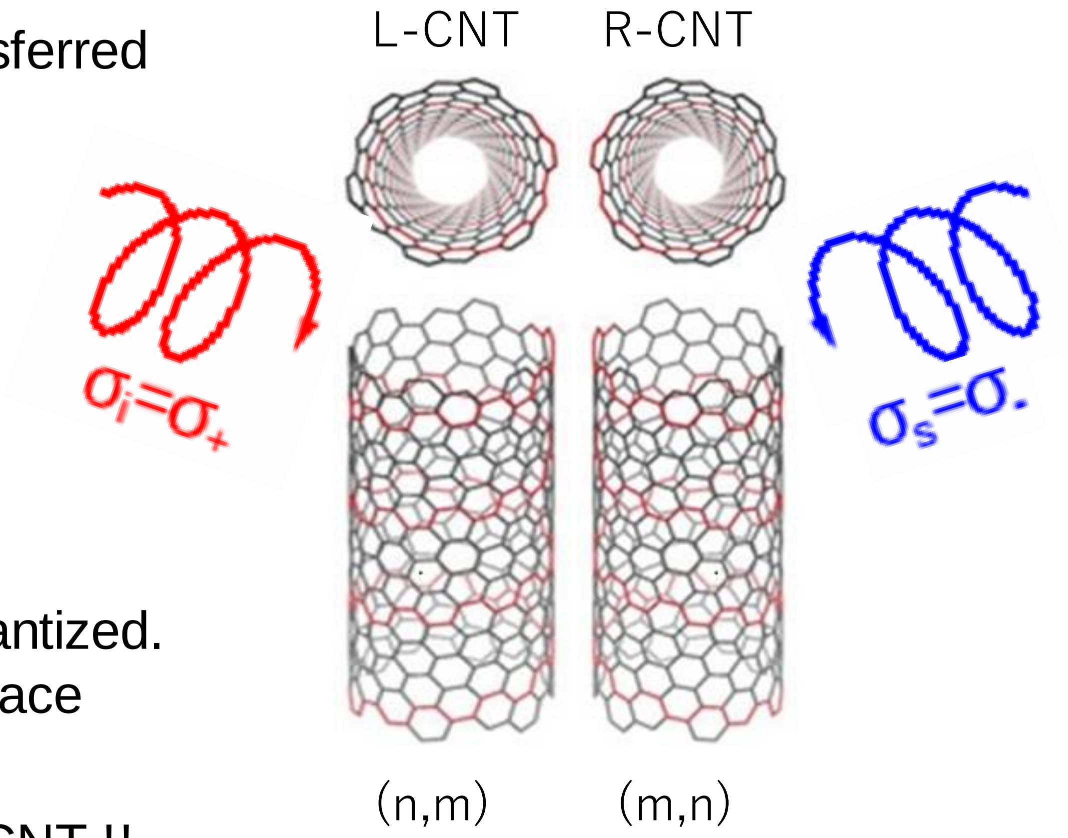


Angular momentum L is transferred from a photon to CNT

$\sigma_+ \ (\triangle L = 1)$

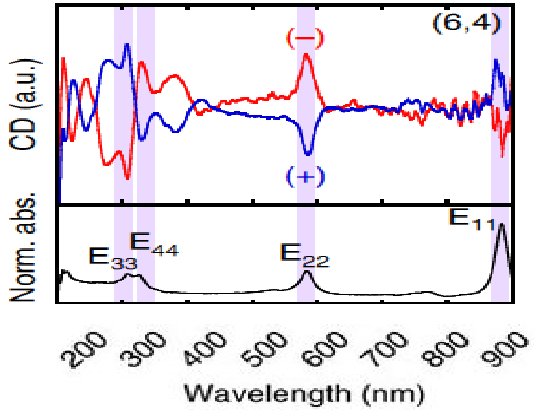
$\sigma_- \ (\triangle L = -1)$

For a given initial state,
final states are different!



Chirality ⇔ CD

Exp.



Circumferential wavevector is quantized.
Cutting lines of nanotubes in k space

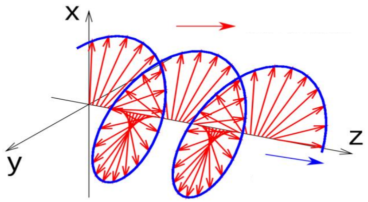
We can separate L-CNT and R-CNT !!

X. Wei et al.
Nat. Comm. 7 12899 (2016)

Δ :Difference of on-site energy of A and B atoms

When we change Δ , VP and PP occurs.

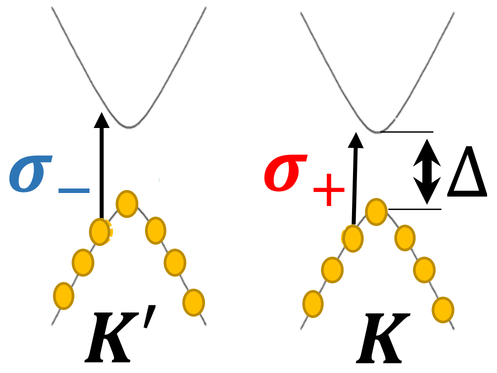
Y. Tatsumi et al, *Phys. Rev. B,* **94**, 235408 (2016)

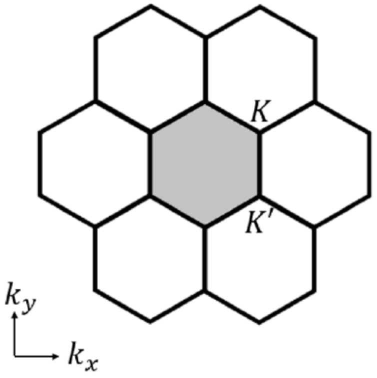


Left-handed (σ_+)
Right-handed (σ_-)

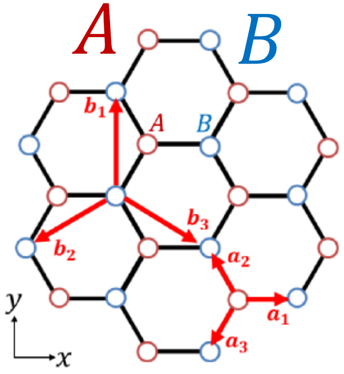
Valley Polarization (VP)

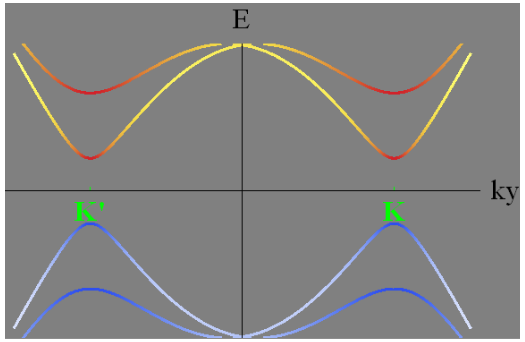
optical absorption at K or K’





Pseudo-spin Polarization (PP)





A ○ $\Delta/2$
B ○ $-\Delta/2$

$$\Psi(k) = C_A(k)\Phi_A(k,r) + C_B(k)\Phi_B(k,r)$$

No VP, PP $(A = B)$
- graphene
- silicene

$\Delta = 0$

vs

VP, PP $(A \neq B)$
- h-BN
- TMD

$\Delta \neq 0$

Why?

TMD: transition metal dichalcogenides

Question

Δ:Difference of on-site energy of A & B

No VP, PP $(A = B)$

graphene
silicene
$\Delta = 0$

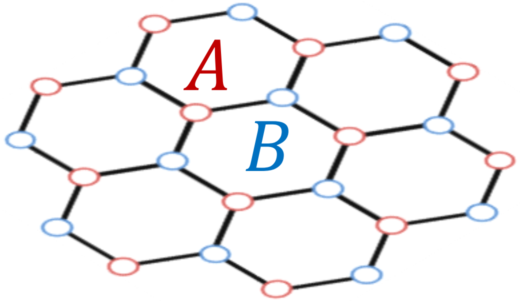
vs

VP, PP $(A \neq B)$

h-BN
TMD
$\Delta \neq 0$

Valley Polarization (VP)

Pseudo-spin Polarization (PP)



○ $\Delta/2$
○ $-\Delta/2$

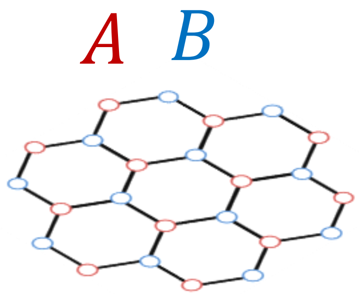
- Are the VP and PP change continuously at $\Delta = 0$?
  - No, there is a *discontinuous* change at $\Delta = 0$.

- Do VP and PP behave simultaneously for $\Delta \neq 0$?
  - Not always, ⇒ the case of Haldane model.

Why?

○ $\Delta/2$
○ $-\Delta/2$

Why are these questions interesting?



No VP, PP ($A = B$)
graphene
silicene
$\Delta = 0$

vs

VP, PP ($A \neq B$)
h-BN
TMD
$\Delta \neq 0$

Why important?

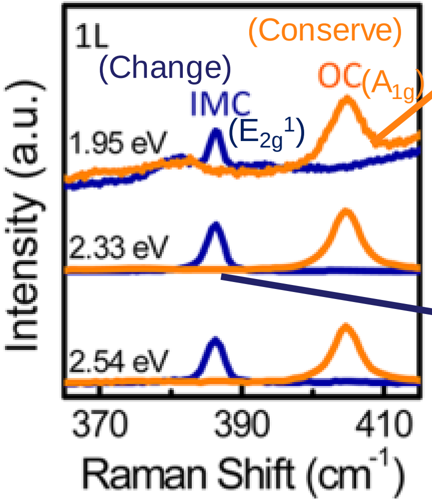
Relevant to

- Fundamental for optical properties of 2D materials
  - CD, Raman, PL, excitons, etc
- Topological properties of 2D materials
  - Inversion of energy bands (spin-orbit interaction)
  - Edge states, Berry phase, Quantum Hall effect etc.
- Symmetry
  - mirror, inversion, time-reversal, charge conjugation

Raman scattering by circularly polarized light

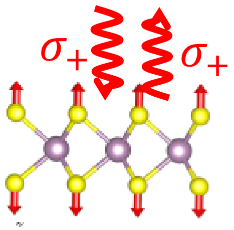
Y. Tatsumi et al, *Phys. Rev. B,* **97**, 195444 (2018) & 115407 (2018)

Monolayer MoS_2



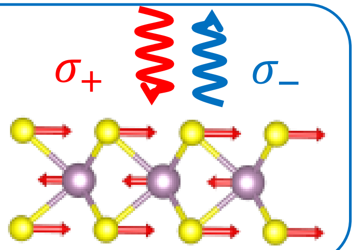
Helicity conserves

OC mode:
Out-of-plane Chalcogen



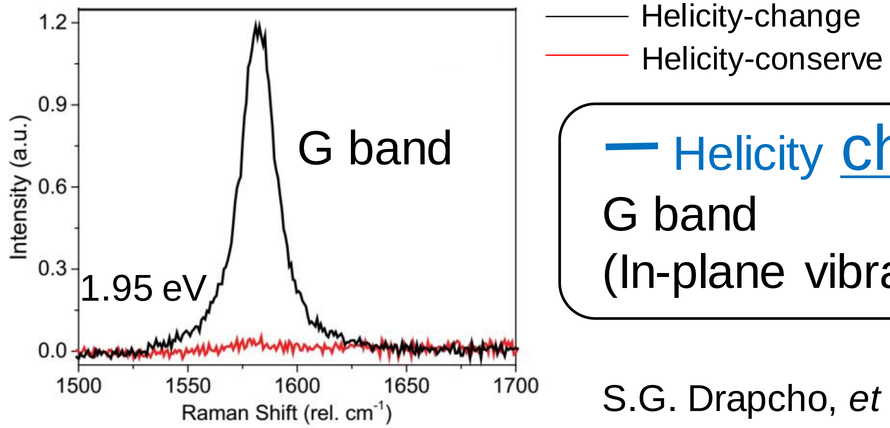
Helicity changes

IMC mode:
In-plane Metal & Chalcogen
(degenerate : x and y)



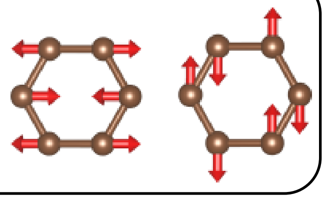
S.-Y. Chen, *et al*., Nano Lett., 15, 2526 (2015)

Graphene



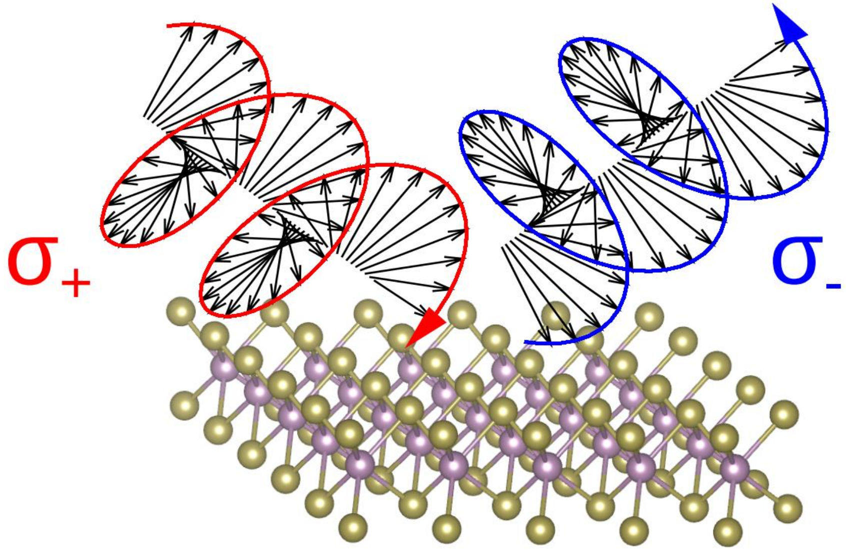
Helicity changes

G band
(In-plane vibration)



S.G. Drapcho, *et al.*, Phys. Rev. B 95, 165417 (2017)

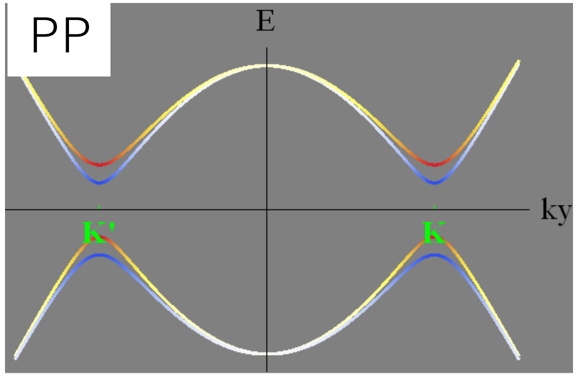
Why?



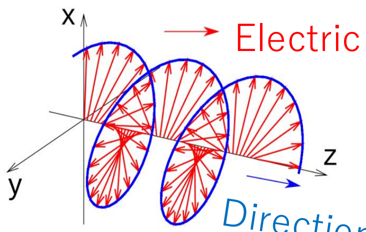
Conservation law of
Angular momentum

Symmetries and Optical properties

- Broken Mirror symmetry (left-handed and right-handed)
  - CD (circular dichroism) occurs
- Broken Inversion symmetry (A and B atoms)
  - VP (valley polarization) occurs
  - PP (pseudo-spin polarization) occurs, edge states
- Spin-orbit interaction
  - Inversion of energy bands (topological insulator)
  - Inversion of VP and PP occurs
- Broken time-reversal symmetry (K and K' points)
  - Large CD (circular dichroism) occurs



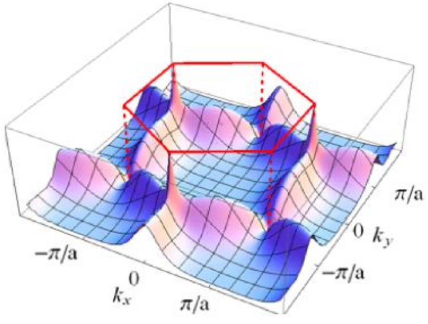
Inversion of energy bands



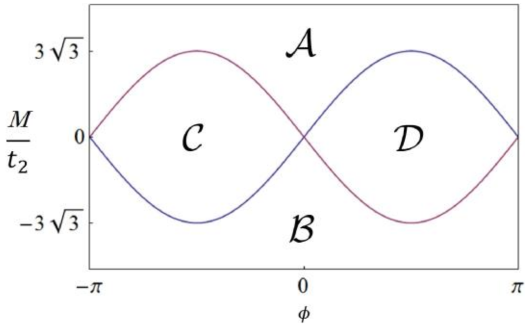
Outline (Let's discuss CD, VP, PP)

SATL
Science of Atomic Layers

1. Change Δ (Graphene, h-BN, silicene, Bi)
   - Discontinuous change of VP and PP at Δ=0
   - VP and PP behave similarly

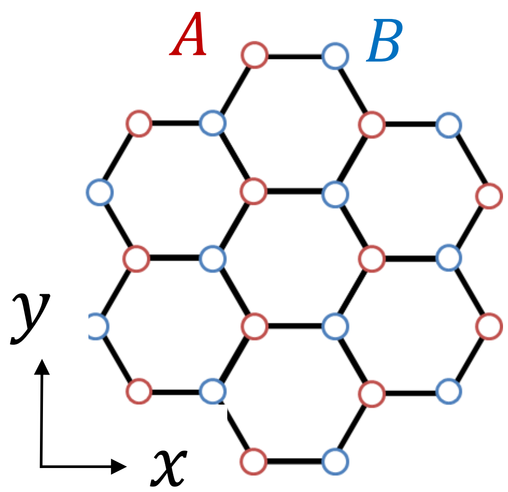


2. the Haldane model (lack of time-reversal symmetry)
   - Perfect CD occurs
   - VP and PP behave independently!



CD: circular dichroism, VP: valley polarization, PP: pseudo-spin polarization

Changing Δ (Graphene, h-BN)



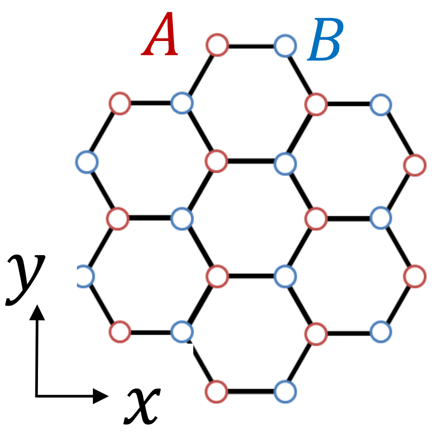
Difference of on-site energy between of A and B atoms

○ $-\Delta/2$ ○ $\Delta/2$

$w(\boldsymbol{k}) = |f(\boldsymbol{k})|$

Graphene ($\boldsymbol{\Delta}$=0) and h-BN ($\Delta \neq 0$)

○ $\Delta/2$ ○ $-\Delta/2$



Hamiltonian

$$H = \begin{pmatrix} \Delta/2 & tf(\boldsymbol{k}) \\ tf(\boldsymbol{k})^* & -\Delta/2 \end{pmatrix}$$

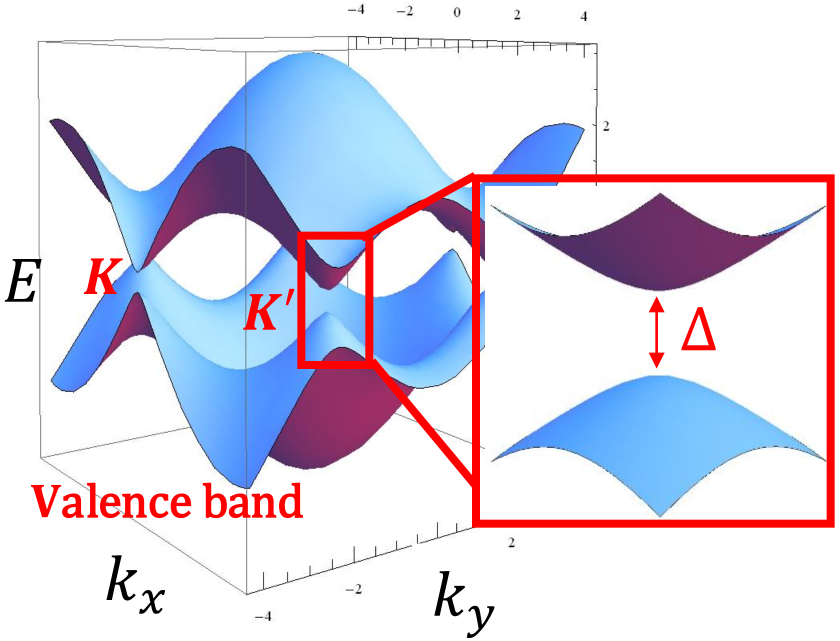
$$H\boldsymbol{C} = E\boldsymbol{C}$$

Wave function

$$\boldsymbol{C}(\boldsymbol{k}) = \begin{pmatrix} C_A(\boldsymbol{k}) \\ C_B(\boldsymbol{k}) \end{pmatrix}$$

	Conduction band	Valence band
Energy	$E^c(\boldsymbol{k}) = \sqrt{\frac{\Delta^2}{4} + t^2 w(\boldsymbol{k})^2}$	$E^v(\boldsymbol{k}) = -\sqrt{\frac{\Delta^2}{4} + t^2 w(\boldsymbol{k})^2}$
PP at K, K’	$\boldsymbol{C}^c(\boldsymbol{K}) = \boldsymbol{C}^c(\boldsymbol{K}') = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\boldsymbol{C}^v(\boldsymbol{K}) = \boldsymbol{C}^v(\boldsymbol{K}') = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Conduction band



PP at K, K’ does not depend on Δ

$$\tan p = \frac{|C_A^d|^2 - |C_B^d|^2}{|C_A^d|^2 + |C_B^d|^2}$$

Wavefunction

$\lambda = c \text{ or } v$

$s = A \text{ or } B$

$$\Psi^\lambda(\boldsymbol{k}, \boldsymbol{r}) = C_A^\lambda(\boldsymbol{k})\Phi_A(\boldsymbol{k}, \boldsymbol{r}) + C_B^\lambda(\boldsymbol{k})\Phi_B(\boldsymbol{k}, \boldsymbol{r})$$

$$\Phi_s(\boldsymbol{k}, \boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R_s}} e^{i\boldsymbol{k}\cdot\boldsymbol{R_s}} \underline{\varphi_s(\boldsymbol{r} - \boldsymbol{R_s})}$$

atomic orbital

N # of unit cell

$\boldsymbol{R_s}$ position of atom

Optical absorption

Hamiltonian

$$\mathcal{H}_{opt} = \frac{i\hbar e}{m}\boldsymbol{A}\cdot\boldsymbol{\nabla} = \frac{\hbar e}{\omega m}\sqrt{\frac{I}{c\varepsilon_0}}e^{i(\boldsymbol{k}_L\cdot\boldsymbol{r}-\omega t)}\boldsymbol{e}_{\boldsymbol{p}}\cdot\boldsymbol{\nabla}$$

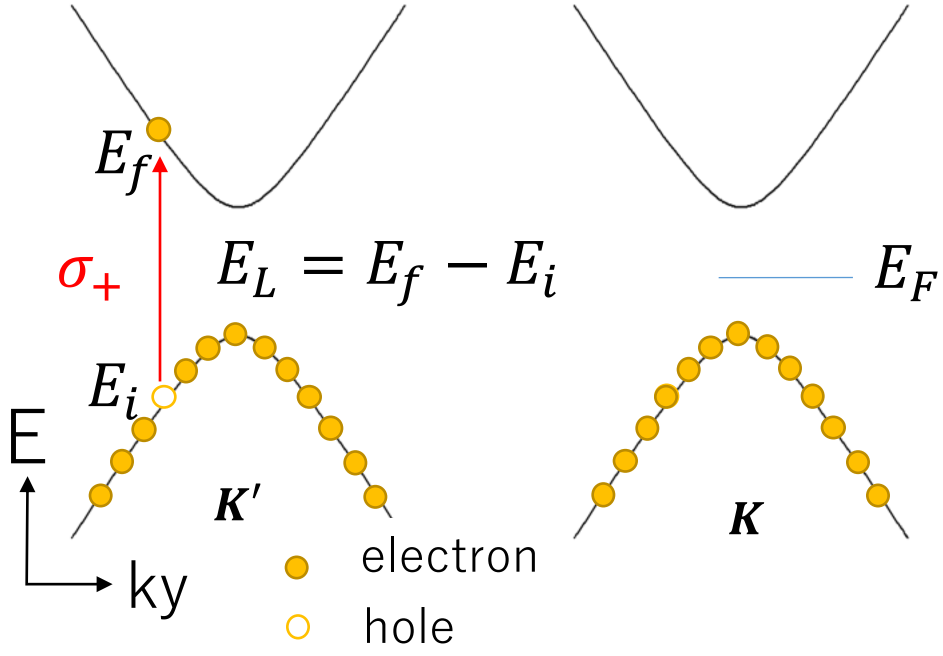
Polarization vector

Transition probability

$$W_{i\to f} \propto \left|\boldsymbol{e}_{\boldsymbol{p}\sigma}\cdot\boldsymbol{D}(\boldsymbol{k})\right|^2$$

Polarization vector・Dipole vector

$$P_+ \propto \begin{pmatrix}1\\ i\\ 0\end{pmatrix}$$



Fermi's golden rule

$$W_{i\to f} = \frac{2\pi}{\hbar}\,|M_{i\to f}|^2\,\delta(E_L - E_f + E_i)$$

Transition matrix element

$$M_{i\to f} = \langle f|\mathcal{H}_{opt}|i\rangle = \left\langle f\left|\frac{\hbar e}{\omega m}\sqrt{\frac{I}{c\varepsilon_0}}e^{i(\boldsymbol{k}_L\cdot\boldsymbol{r}-\omega t)}\boldsymbol{e}_{\boldsymbol{p}}\cdot\boldsymbol{\nabla}\right|i\right\rangle \propto \boldsymbol{e}_{\boldsymbol{p}}\cdot\langle f|\boldsymbol{\nabla}|i\rangle$$

$$= \boldsymbol{D}_{i\to f}(\boldsymbol{k})$$

Dipole vector

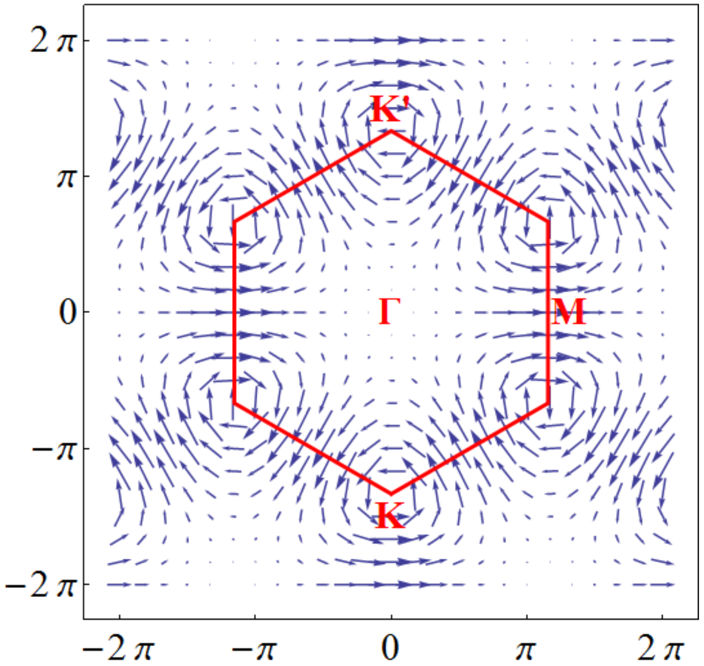
E_L: energy of light
E_i: energy of initial state
E_f: energy of final state
$|i\rangle$: initial state
$|f\rangle$: final state

Dipole vector of graphene

A. Gruneis et al. *Phys. Rev.* B 67, 165402 (2003)

$$\langle \varphi_B(\boldsymbol{r}-\boldsymbol{R}_j)|\boldsymbol{\nabla}|\varphi_A(\boldsymbol{r})\rangle = -\frac{\sqrt{3}}{a} m_{opt}\boldsymbol{R}_j$$

$\boldsymbol{D}_{i\to f}(\boldsymbol{k})$ is a Real vector !!



$$\boldsymbol{D}_{i\to f}(\boldsymbol{k}) = -\frac{\sqrt{3}}{a} m_{opt} 2\mathrm{Re}\left[C_B^c(\boldsymbol{k})^* C_A^v(\boldsymbol{k}) \sum_{j=1}^{3} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_j}\boldsymbol{R}_j \right]$$

$$\boldsymbol{D}_{i\to f}(\boldsymbol{k}) = \begin{pmatrix} D_x(\boldsymbol{k}) \\ D_y(\boldsymbol{k}) \end{pmatrix} \qquad D_x, D_y \in \mathbb{R}$$

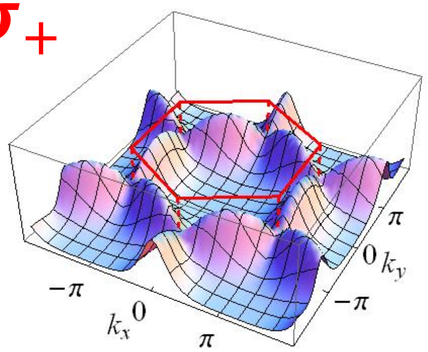
$$W_{i\to f} \propto \left|\boldsymbol{e}_{p\sigma}\cdot\boldsymbol{D}(\boldsymbol{k})\right|^2 = \left|\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \sigma i\end{pmatrix}\cdot\begin{pmatrix}D_x\\ D_y\end{pmatrix}\right|^2 = \frac{1}{\sqrt{2}}\left|D_x - i\sigma D_y\right|^2$$

$$\boldsymbol{e}_{p\sigma} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \sigma i\end{pmatrix}$$

$$= \frac{1}{\sqrt{2}}\left(D_x^2 + \sigma^2 D_y^2\right) = \frac{1}{\sqrt{2}}\left(D_x^2 + D_y^2\right)$$

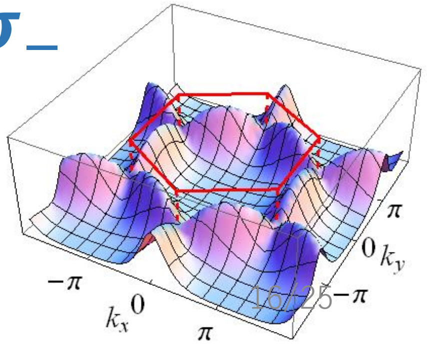
$$\sigma = \begin{cases} +1\ (\sigma_+) \\ -1\ (\sigma_-) \end{cases}$$

$\boldsymbol{\sigma_+}$



=

$\boldsymbol{\sigma_-}$



Graphene: No CD, No VP, No PP

Dipole vector of h-BN

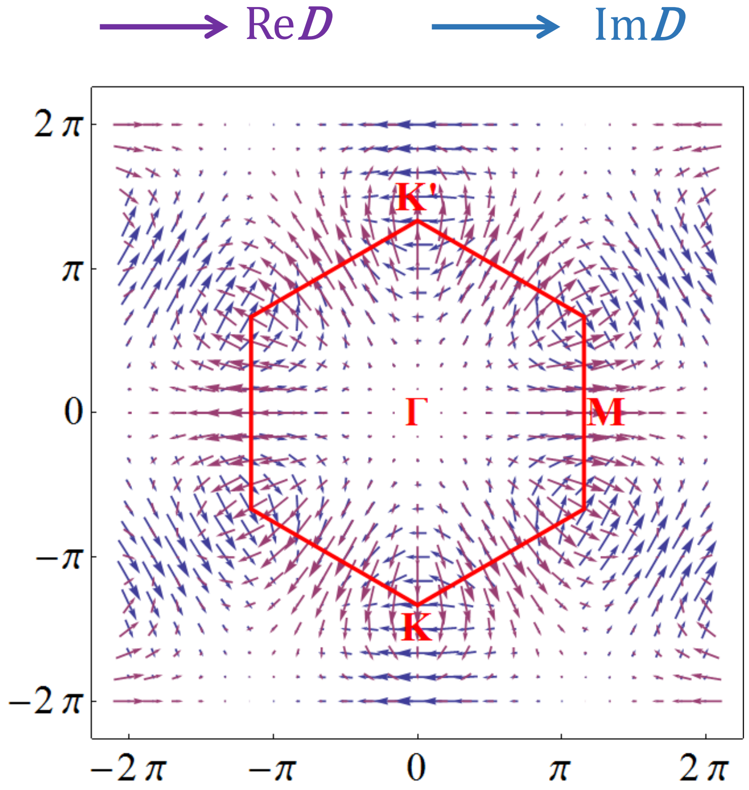
K. Ghalamkari et al, *J. Phys. Soc. Jpn.* **87**, 024710 (2018)

$$\langle \varphi_B(\boldsymbol{r}-\boldsymbol{R}_j)|\boldsymbol{\nabla}|\varphi_A(\boldsymbol{r})\rangle = -\frac{\sqrt{3}}{a} m_{opt} \boldsymbol{R}_j$$

No symmetry between A and B.

$$\boldsymbol{D}_{i\to f}(\boldsymbol{K}) = \frac{3}{2} m_{opt} \left\{ C_A^c(\boldsymbol{K})^* C_B^v(\boldsymbol{K}) \begin{pmatrix} 1 \\ -i \end{pmatrix} - C_B^c(\boldsymbol{K})^* C_A^v(\boldsymbol{K}) \begin{pmatrix} 1 \\ i \end{pmatrix} \right\}$$

$\boldsymbol{D}_{i\to f}(\boldsymbol{k})$ is a Complex vector !!



At $\boldsymbol{K}$ point

$$\boldsymbol{D}_{i\to f}(\boldsymbol{K}) = -\frac{3}{2} m_{opt} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

At $\boldsymbol{K}'$ point

$$\boldsymbol{D}_{i\to f}(\boldsymbol{K}') = -\frac{3}{2} m_{opt} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

σ_+:

$$\boldsymbol{e}_{p+} \cdot \boldsymbol{D}_{i\to f}(\boldsymbol{K}) \propto \begin{pmatrix} 1 \\ i \end{pmatrix} \cdot \begin{pmatrix} 1 \\ i \end{pmatrix} = 2 \qquad \boldsymbol{e}_{p+} \cdot \boldsymbol{D}_{i\to f}(\boldsymbol{K}') \propto \begin{pmatrix} 1 \\ i \end{pmatrix} \cdot \begin{pmatrix} 1 \\ -i \end{pmatrix} = 0$$

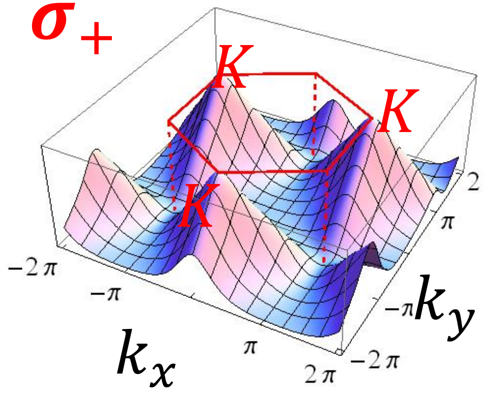
σ_-:

$$\boldsymbol{e}_{p-} \cdot \boldsymbol{D}_{i\to f}(\boldsymbol{K}) \propto \begin{pmatrix} 1 \\ -i \end{pmatrix} \cdot \begin{pmatrix} 1 \\ i \end{pmatrix} = 0 \qquad \boldsymbol{e}_{p-} \cdot \boldsymbol{D}_{i\to f}(\boldsymbol{K}') \propto \begin{pmatrix} 1 \\ -i \end{pmatrix} \cdot \begin{pmatrix} 1 \\ i \end{pmatrix} = 2$$

$$\boldsymbol{e}_{p\sigma} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \sigma i \end{pmatrix}$$

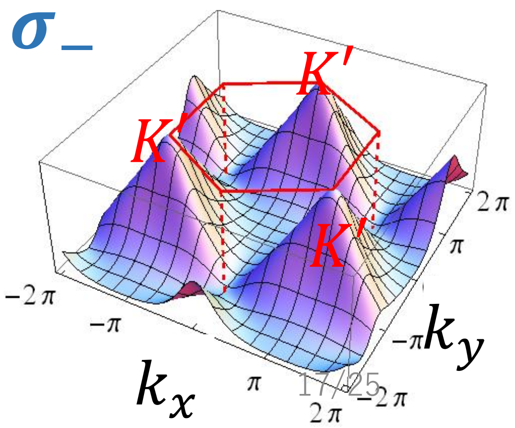
$$\sigma = \begin{cases} +1 \ (\sigma_+) \\ -1 \ (\sigma_-) \end{cases}$$

σ_+



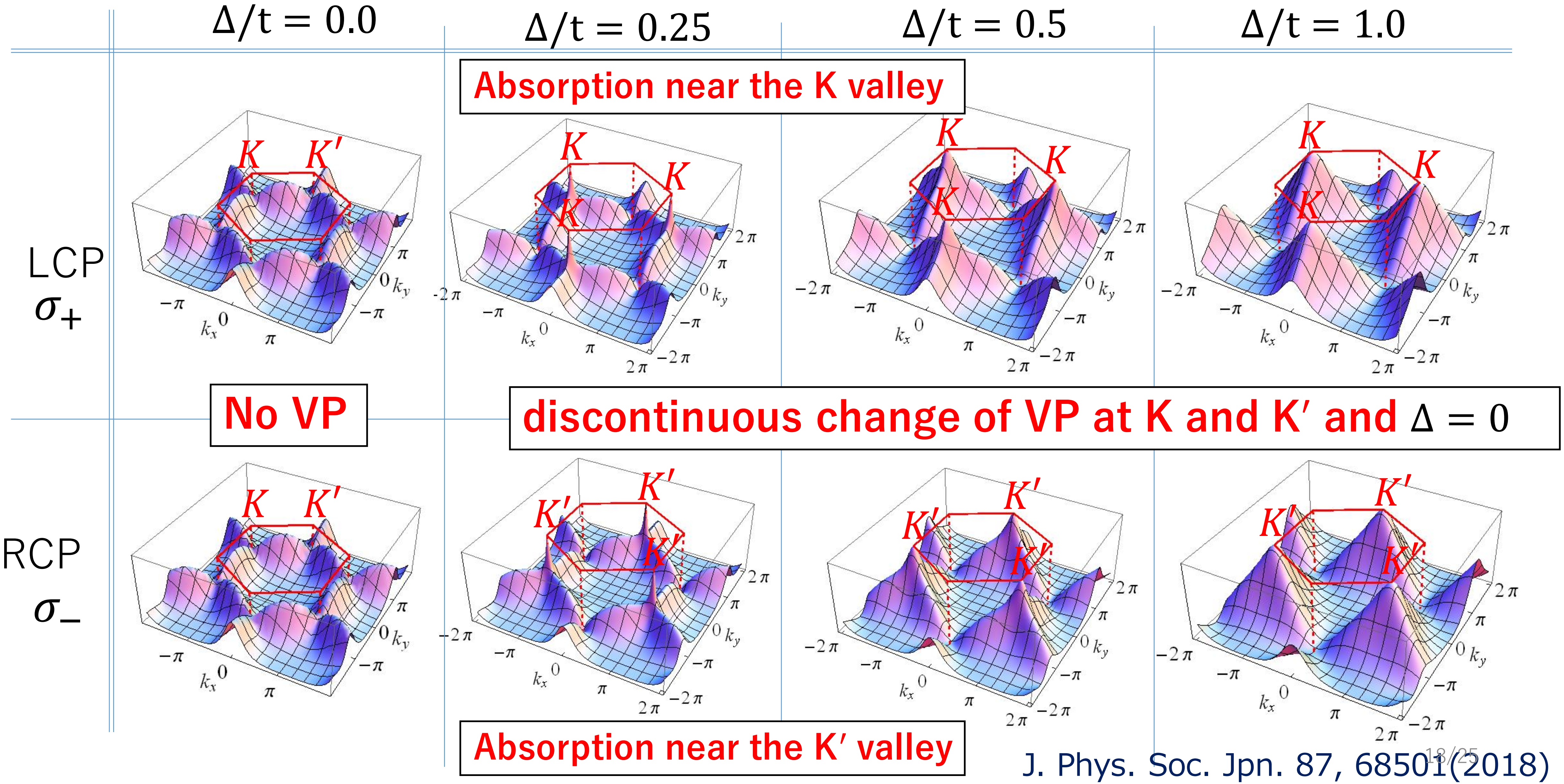
≠

σ_-



h-BN: No CD, Yes VP, Yes PP

Δ dependence of absorption matrix element, $\boldsymbol{e_p} \cdot \boldsymbol{D_{i\rightarrow f}}$



J. Phys. Soc. Jpn. 87, 68501(2018)

Integration on k for given E_L

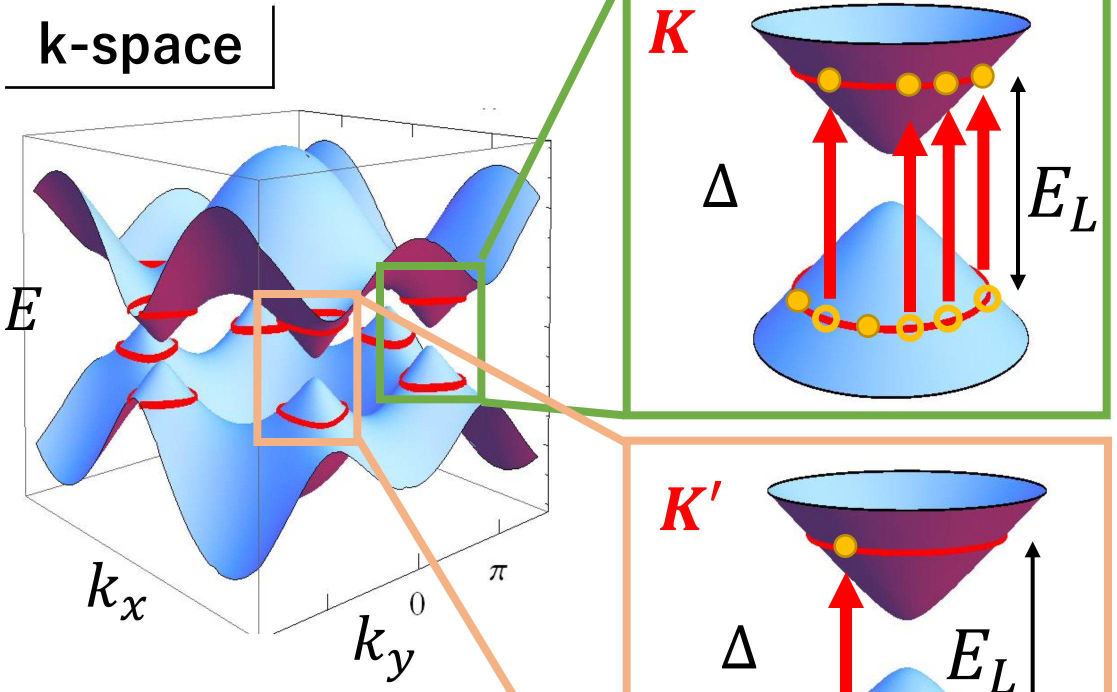
Degree of valley polarization

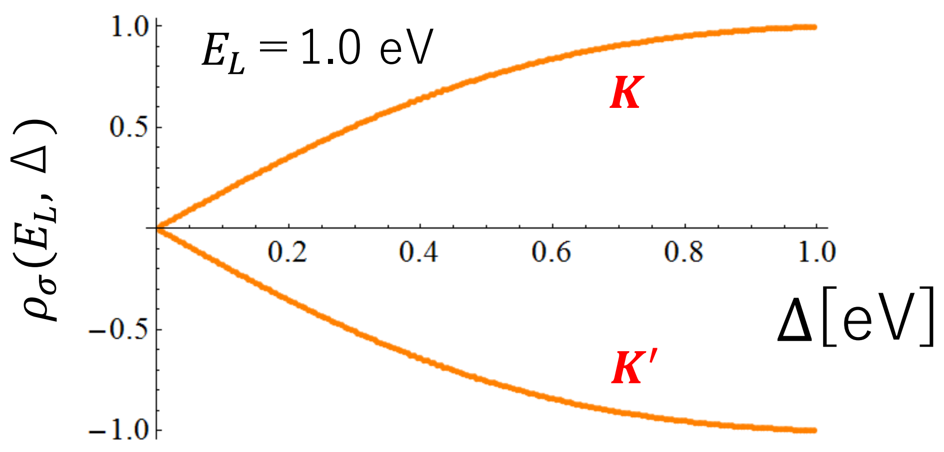
For given E_L

$$\rho_\sigma(E_L, \Delta) = \frac{I_\sigma[K] - I_\sigma[K']}{I_\sigma[K] + I_\sigma[K']}$$

$$I_\sigma[K] = \int_{C_K} d\boldsymbol{k} |\boldsymbol{e}_{p\sigma} \cdot \boldsymbol{D}(\boldsymbol{k})|^2 \quad I_\sigma[K'] = \int_{C_{K'}} d\boldsymbol{k} |\boldsymbol{e}_{p\sigma} \cdot \boldsymbol{D}(\boldsymbol{k})|^2$$

Equi-energy line around K point   around K' point

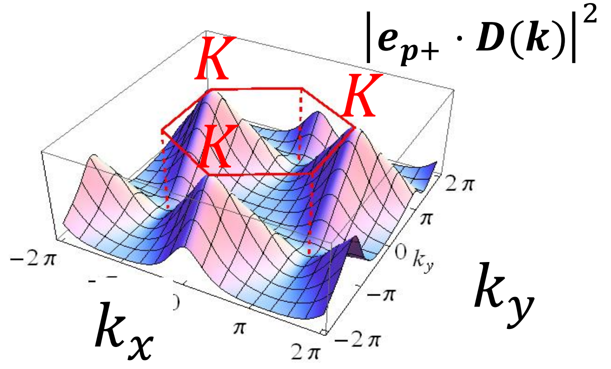




If $E_L = \Delta$, transition occurs only at K and K', then

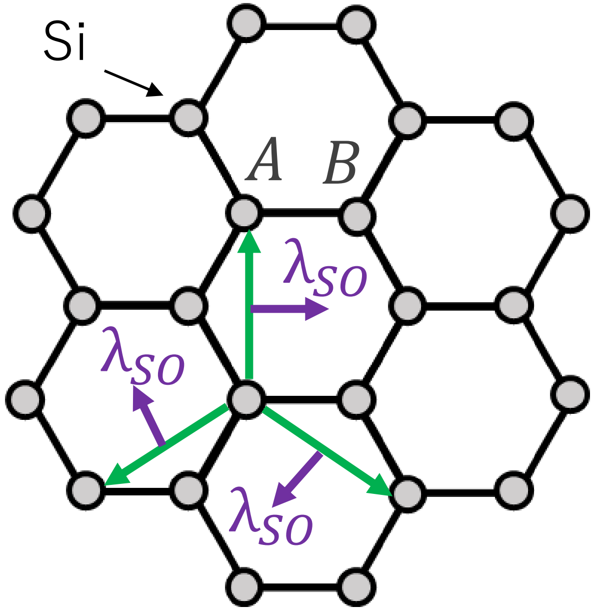
$$\tan V = \frac{I_\sigma(K) - I_\sigma(K')}{I_\sigma(K) + I_\sigma(K')} = 1 \text{ or } -1$$

for any Δ except for Δ=0.

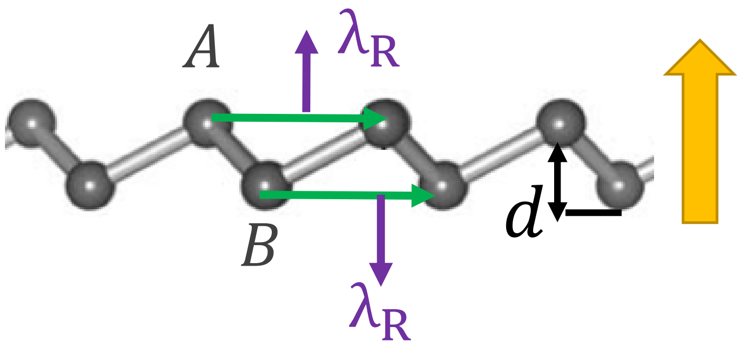


$\rho_\sigma(E_L, \Delta)$ changes monotonically for a fix E_L with increasing Δ !!

Changing Δ (silicene)



Δ can be changed by applying E_z



$$eE_z d = \pm\Delta/2$$

Energy band of silicene with changing **Δ**

Hamiltonian

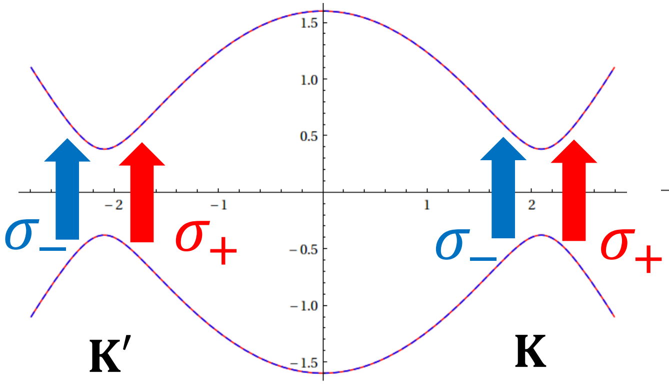
$$H = \begin{pmatrix} \lambda_{SO}(\boldsymbol{k}) + \Delta/2 & tf(\boldsymbol{k}) & \lambda_R(\boldsymbol{k}) & 0 \\ tf(\boldsymbol{k})^* & -\lambda_{SO}(\boldsymbol{k}) - \Delta/2 & 0 & -\lambda_R(\boldsymbol{k}) \\ \lambda_R(\boldsymbol{k})^* & 0 & -\lambda_{SO}(\boldsymbol{k}) + \Delta/2 & tf(\boldsymbol{k}) \\ 0 & -\lambda_R(\boldsymbol{k})^* & tf(\boldsymbol{k})^* & \lambda_{SO}(\boldsymbol{k}) - \Delta/2 \end{pmatrix}$$

Columns: $\uparrow A$, $\uparrow B$, $\downarrow A$, $\downarrow B$; rows: $\uparrow A$, $\uparrow B$, $\downarrow A$, $\downarrow B$

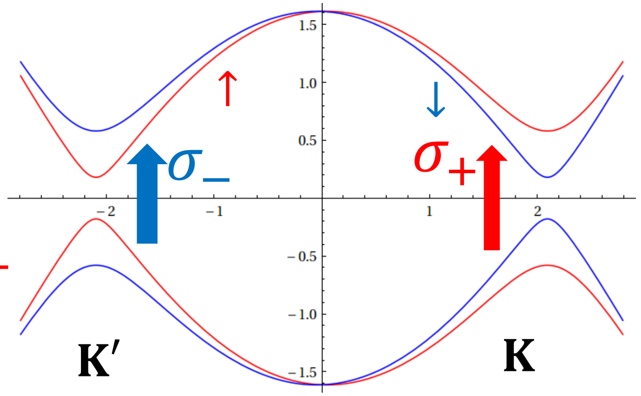
Energy dispersion

$$E(\boldsymbol{k}) = \pm\sqrt{\lambda_{SO}(\boldsymbol{k})^2 + \left(\frac{\Delta}{2}\right)^2 + \lambda_R(\boldsymbol{k})\lambda_R(\boldsymbol{k})^* + t^2 f(\boldsymbol{k})f(\boldsymbol{k})^* \pm \Delta\sqrt{\lambda_{SO}(\boldsymbol{k})^2 + \lambda_R(\boldsymbol{k})\lambda_R(\boldsymbol{k})^*}}$$

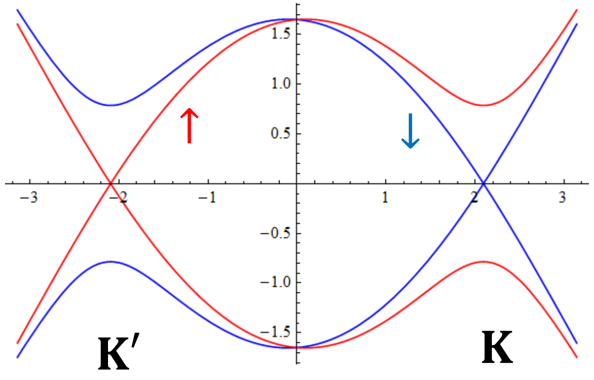
$\frac{\Delta}{2} = 0$



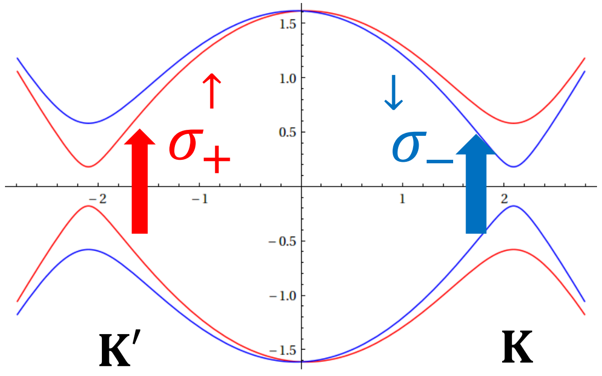
$0 < \frac{\Delta}{2} < \lambda_{SO}$



$\frac{\Delta}{2} = \lambda_{SO}$



$\frac{\Delta}{2} > \lambda_{SO}$



Energy band gap $= 2\lambda_{SO}(\boldsymbol{K})$

$\lambda_{SO}(\boldsymbol{K}) = -\lambda_{SO}(\boldsymbol{K}')$

$\lambda_R(\boldsymbol{K}) = \boldsymbol{0}$

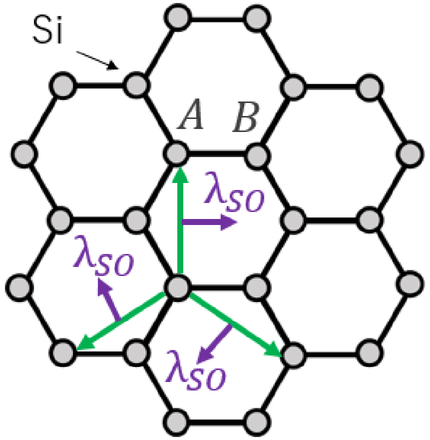
$f(\boldsymbol{K}) = 0$

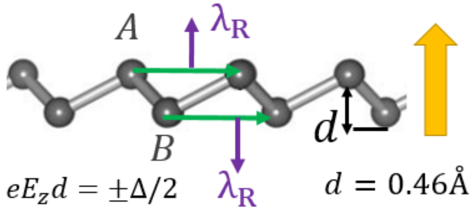
$E_z = 17\ \mathrm{meV/Å}$

$eE_z d = \pm\Delta/2$

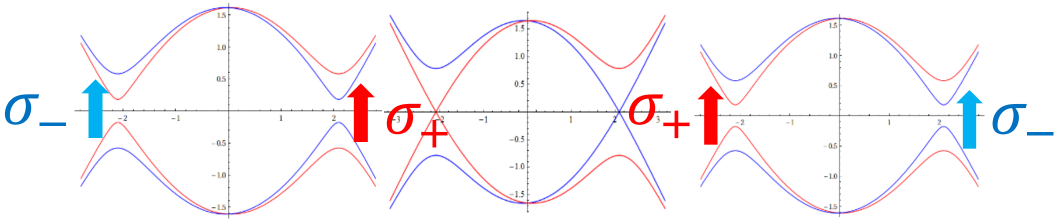
Silicene: transition from topological to band-gap insulator

K. Ghalamkari *et al.*, *J. Phys. Soc. Jpn.* **87**, 024710 (2018)

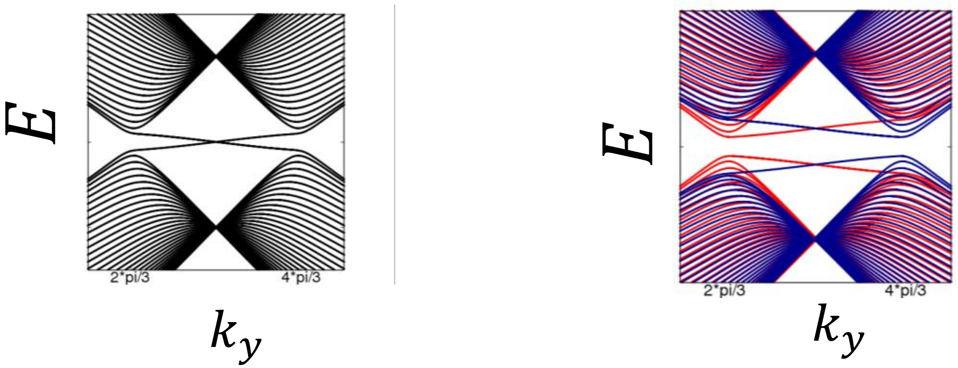




$0 < \frac{\Delta}{2} < \lambda_{so}$ $\qquad \frac{\Delta}{2} = \lambda_{so}$ $\qquad \frac{\Delta}{2} > \lambda_{so}$

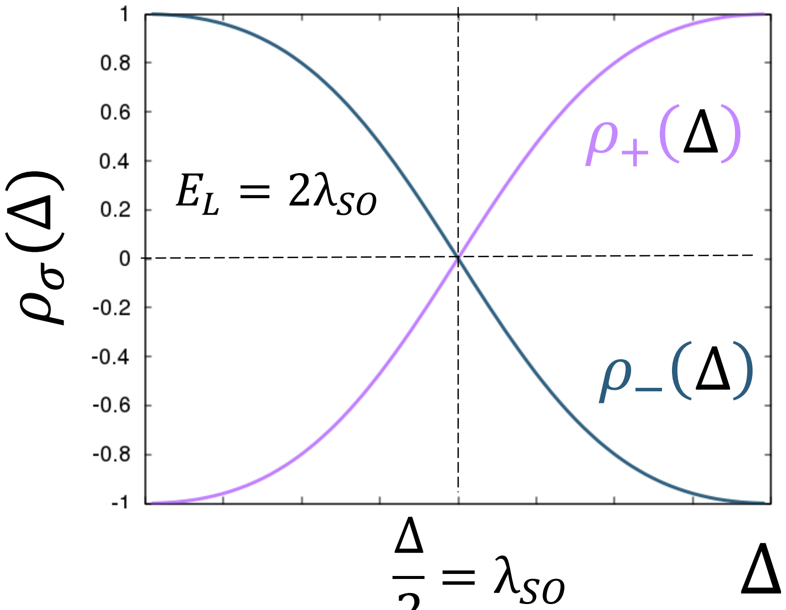


topological insulator | Semimetal | band-gap insulator



Energy band of Si *nanoribbon*

VP changes the sign



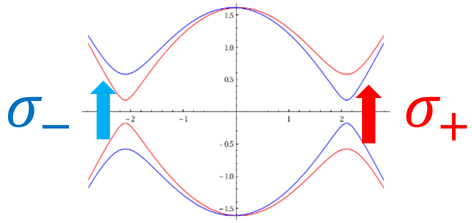
$$\rho_\sigma(\Delta) = \frac{I_\sigma[K] - I_\sigma[K']}{I_\sigma[K] + I_\sigma[K']}$$

M.Ezawa Phys.Rev. **B** 86, 161407(2012)

Pseudospin Polarization (PP) of silicene

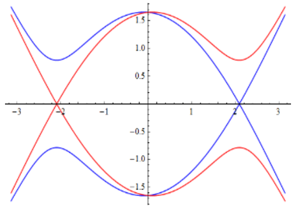
VP

$0 < \frac{\Delta}{2} < \lambda_{SO}$



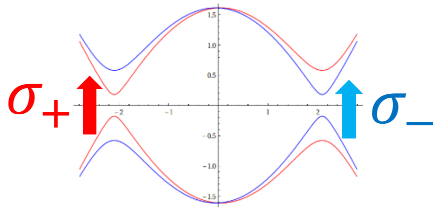
Topological insulator

$\frac{\Delta}{2} = \lambda_{SO}$



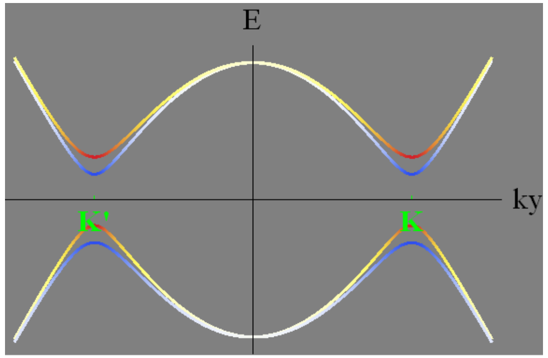
Semimetal

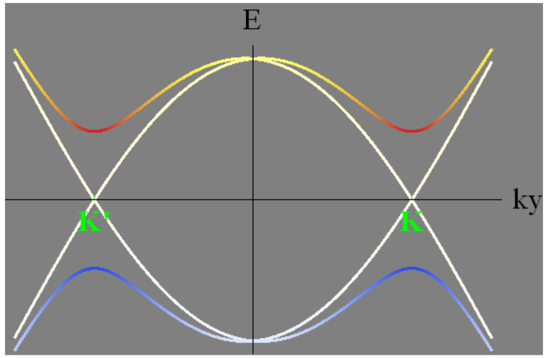
$\frac{\Delta}{2} > \lambda_{SO}$

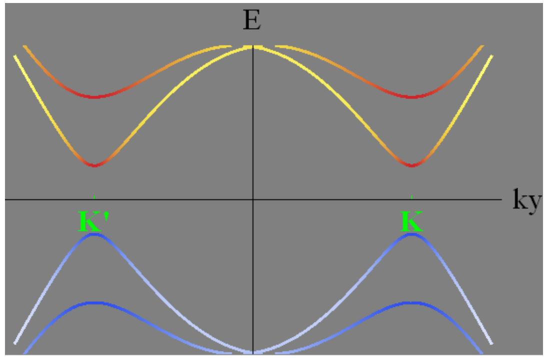


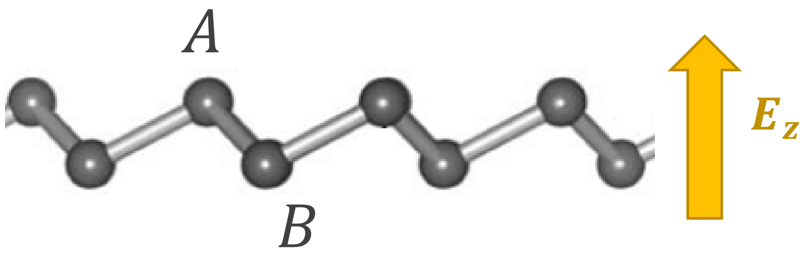
band-gap insulator

PP

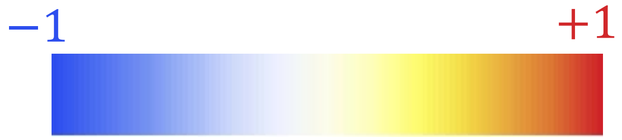






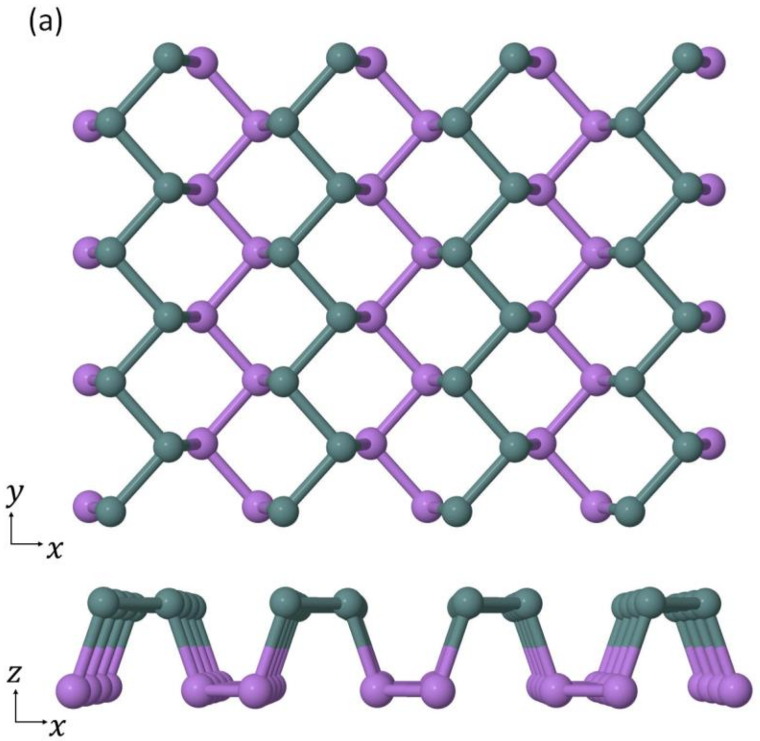


Both VP and PP change the sign!



B atom A atom

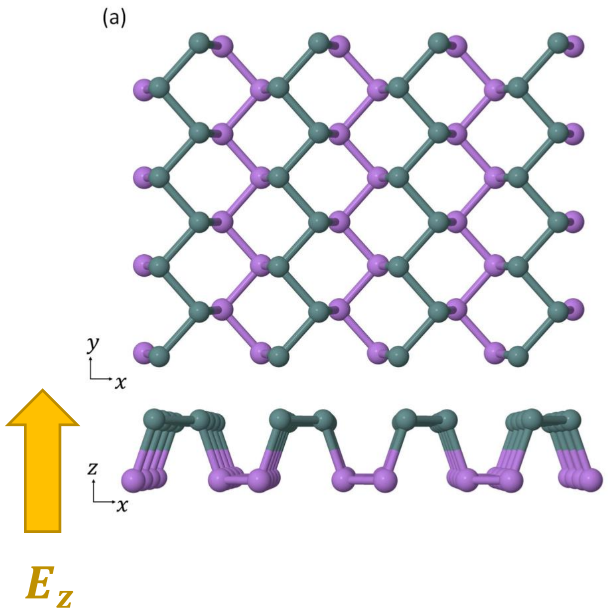
Changing Δ (XY anisotropic 2D material)
Black P, GaTe, Bismuthene



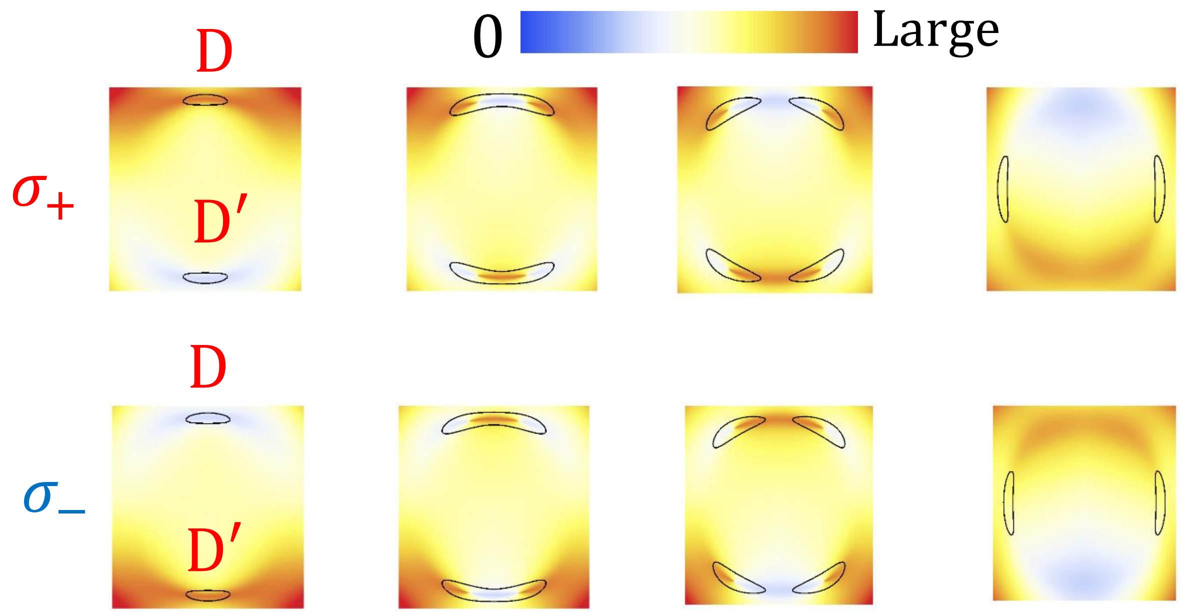
Large spin-orbit interaction
XY Anisotropic buckled structure

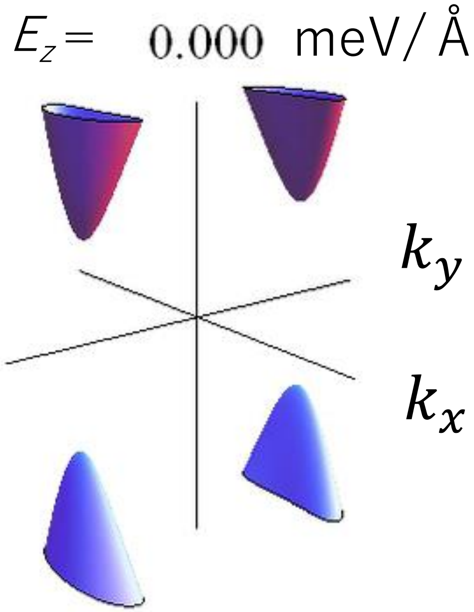
Pseudo Spin is now defined between
Upper layer and lower layer

VP and PP inversion simultaneously occur for Bi



VP

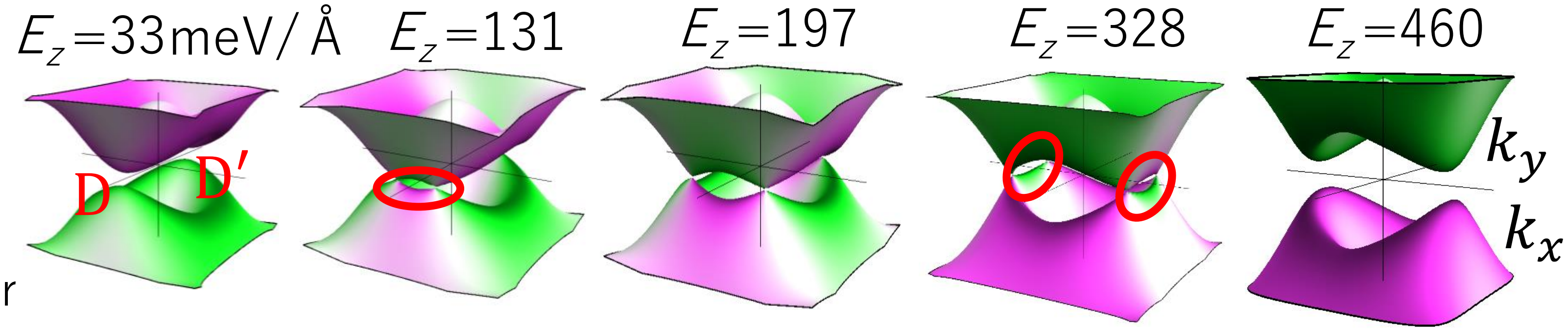




Large spin-orbit
Anisotropic (x, y)

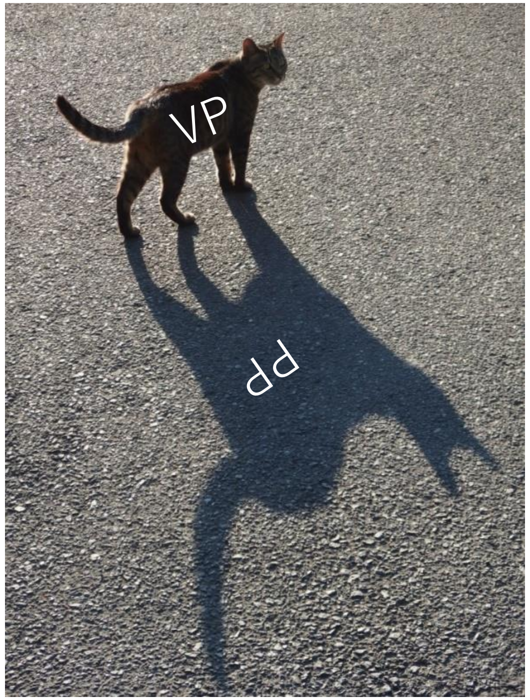
Upper layer Lower layer

PP



Topological ⟵ Semimetal ⟶ band-gap insulator

VP and PP behaves similarly !!



Graphene: No VP and No PP

h-BN: VP and PP exists for $\Delta \neq 0$

Silicene: VP and PP change the sign at $\frac{\Delta}{2} = \lambda_{so}$

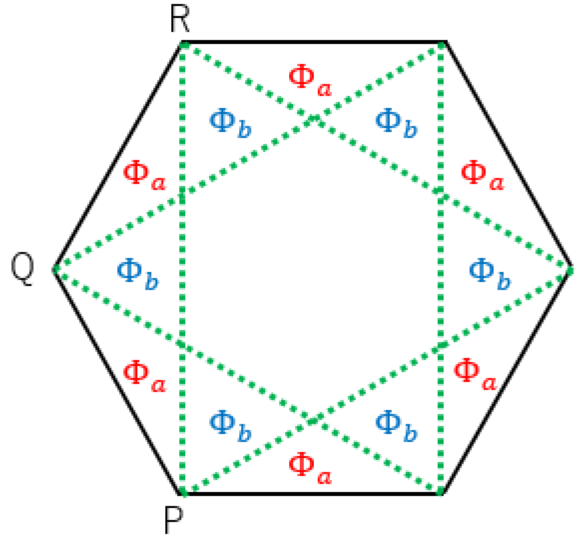
XY: VP and PP change the sign for X and Y

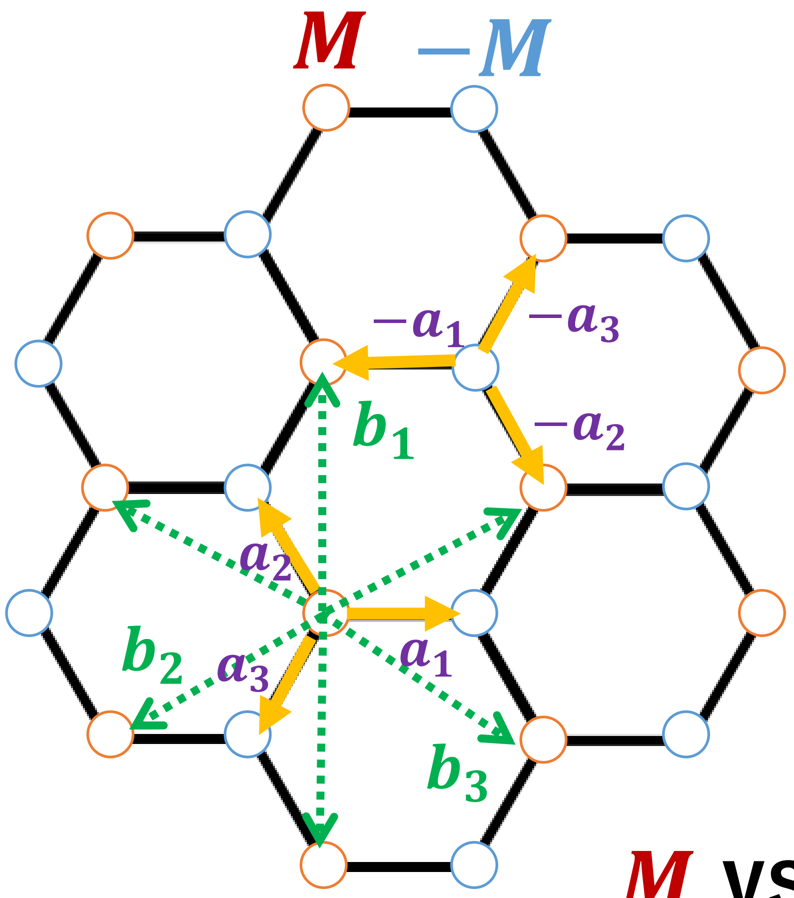
all Hamiltonian's have time-reversal symmetry

Question: Are VP and PP independent? Any interaction?

Changing Δ (=M) (Haldane model)

local magnetic field ϕ





○ M

○ $-M$

Notation by Haldane

Nearest neighbor: t_1

Next nearest neighbtor: t_2

b_1, b_2, b_3 $e^{i\phi} t_2$

$-b_1, -b_2, -b_3$ $e^{-i\phi} t_2$

Phase by local magnetic field

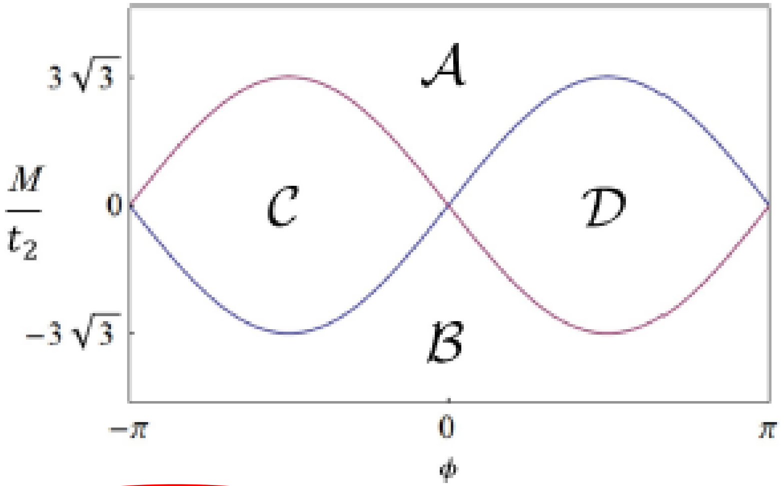
ϕ

M vs ϕ

F. D. M. Haldane, *Phys. Rev. Lett.* 61, 2015 (1988).

Yes! VP and PP are independent

K. Ghalamkari *et al.*, J. Phys. Soc. Jpn. 87, 063708 (2018)



- Broken time-reversal symmetry ($\phi \neq 0$)
- Haldane's model ($M = \Delta$)
  - Center: $M = \phi = 0 \rightarrow$ graphene
  - $\mathcal{A}, \mathcal{B}$: $M \neq 0, \phi = 0 \rightarrow$ h-BN
  - $\mathcal{C}, \mathcal{D}$: $M = 0, \phi \neq 0 \rightarrow$ quantum Hall

Region	$\mathcal{A}$	$\mathcal{B}$	$\mathcal{C}$	$\mathcal{D}$
VP ($\tan V$)	$+1$	-1	0	0
pCD ($\tan \theta$)	0	0	-1	$+1$
PP-c(K, K') ($\tan p$)	$(+1, +1)$	$(-1, -1)$	$(+1, -1)$	$(-1, +1)$
PP-v(K, K') ($\tan p$)	$(-1, -1)$	$(+1, +1)$	$(-1, +1)$	$(+1, -1)$
σ_{xy}	0	0	$+1$	-1

2x2 Hamiltonian of Haldane's model

$$H = \begin{pmatrix} A_0 + A_3 & A_1 - iA_2 \\ A_1 + iA_2 & A_0 - A_3 \end{pmatrix}$$

$$A_0 = 2t_2 \cos\phi \sum_{j=1}^{3} \cos(\boldsymbol{k} \cdot \boldsymbol{b}_j), \quad A_1 = t_1 \sum_{j=1}^{3} \cos(\boldsymbol{k} \cdot \boldsymbol{a}_j),$$

$$A_2 = t_1 \sum_{j=1} \sin(\boldsymbol{k} \cdot \boldsymbol{a}_j), \quad A_3 = -2t_2 \sin\phi \sum_{j=1} \sin(\boldsymbol{k} \cdot \boldsymbol{b}_j) + M,$$

VP occurs for $\mathcal{A}, \mathcal{B}$
PP occurs for all $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$

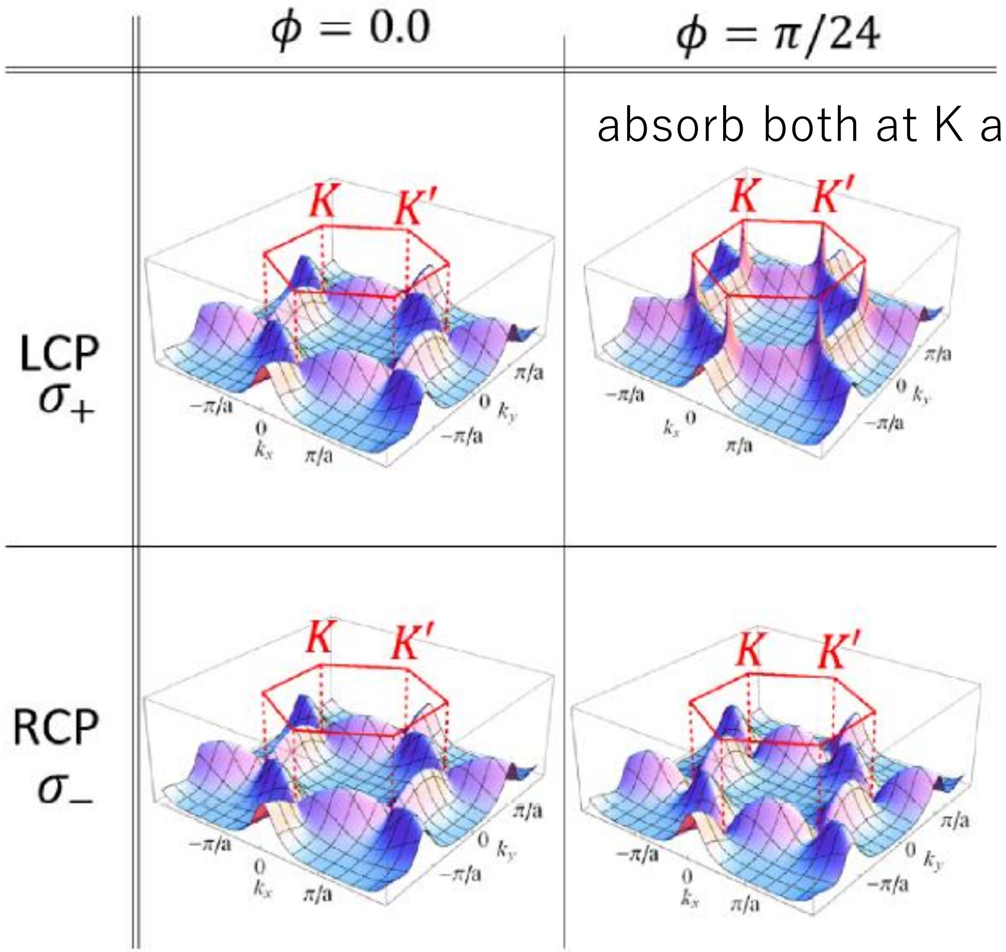
VP: valley polarization

$$\tan V = \frac{I_\sigma(K) - I_\sigma(K')}{I_\sigma(K) + I_\sigma(K')}$$

PP: pseudo-spin polarization

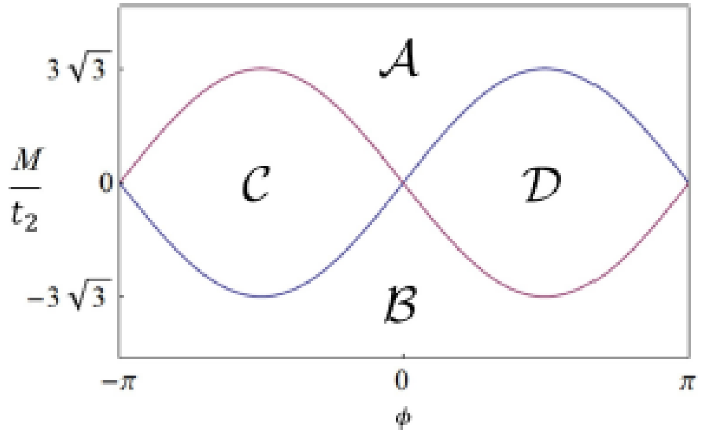
$$\tan p = \frac{|C_A^d|^2 - |C_B^d|^2}{|C_A^d|^2 + |C_B^d|^2}$$

Perfect CD occurs!



absorb both at K and K'

No absorption both at K and K'



For Region $\mathcal{C}$, $\mathcal{D}$ (M=0, $\phi \neq 0$)

No VP, Opposite PP for K and K'

Perfect CD ($\tan\theta = 1$)

absorb only $\boldsymbol{\sigma_+}$

$$\tan\theta = \frac{I(\sigma_+) - I(\sigma_-)}{I(\sigma_+) + I(\sigma_-)}$$

Region	$\mathcal{A}$	$\mathcal{B}$	$\mathcal{C}$	$\mathcal{D}$
VP ($\tan V$)	+1	−1	0	0
pCD ($\tan\theta$)	0	0	−1	+1
PP-c(K, K') ($\tan p$)	(+1, +1)	(−1, −1)	(+1, −1)	(−1, +1)
PP-v(K, K') ($\tan p$)	(−1, −1)	(+1, +1)	(−1, +1)	(+1, −1)
σ_{xy}	0	0	+1	−1

Take Home messages

-We can predict the following optical phenomena !

- Graphene
  - Helicity change Raman for G-band. (Bending ⇒ CD, edge ⇒ PP).
- Silicene (from topological to band-gap insulator)
  - VP and PP changes sign by applying electric field at $E_z = 17\ \mathrm{meV/Å}$
- TMDs
  - Helicity change in Raman can be observed (even applying the strain).
- XY anisotropic 2D materials (Bi, GaTe ⋯)
  - Semi metallic phase appear by applying electric field around 100$\mathrm{meV/Å}$
- Haldane material (α -$(BEDTTTF)_2I_3$. see JPSJ **86**, 123702 (2017))
  - Perfect CD can be observed. Sign change of Berry curvature

Note: Green colored statements are not discussed in this presentation.