

## From Graphene to Silicene: Topological Phase Diagram and Transition

EQPCM Symposium Motohiko Ezawa Department of Applied Physics University of Tokyo

## Outline



- Silicene is a graphene-like silicon structure
- It has a rich variety of topological phases induced by applying various external fields
- They are QSH, QAH, hybrid QSQAH insulators
- There appear topological (semi)metals such as single-Dirac cone state and valley-polarized metal
- DOS & quantized conductance of edge channels
   Experimental observations by STM/STS, ARPES

## Silicene





- •K. Takeda and K. Shiraishi, Phys. Rev. B 50, 075131 (1994).
- •G. G. Guzm´an-Verri and L. C. Lew Yan Voon, Phys. Rev. B 76, 075131 (2007).
- C-C. Liu, W. Feng, and Y. Yao, PRL 107, 076802 (2011)
- C-C. Liu, H.Jiang and Y. Yao, PRB 84 195430 (2011)

## My Works on Silicene

#### 15 papers including 2 PRL

- 1. "Topological Insulator and Helical Zero Mode in Silicene under Inhomogeneous Electric Field,
- 2. "Quantum Hall Effects in Silicene",
- 3. "Quantum Anomalous Hall Effects and Valley-Polarized Metals in Silicene"
- 4. "Dirac Theory and Topological Phases of Silicon Nanotube"
- 5. "Quasi-Topological Insulator and Trigonal Warping in Gated Bilayer Silicene",
- 6. "Topological Phase Transition and Electrically Tunable Diamagnetism in Silicene"
- 7. "Spin-Valley Optical Selection Rule and Strong Circular Dichroism in Silicene"
- 8. "Photo-Induced Topological Phase Transition and Single Dirac-Cone State in Silicene"

### M. Ezawa, New J. Phys. 14, 033003 (2012)M. Ezawa, J. Phys. Soc. Japan 81, 064705 (2012)

- M. Ezawa, Phys. Rev. Lett 109, 055502 (2012)
- M. Ezawa, Europhysics Letters 98, 67001 (2012)
- M. Ezawa, J. Phys. Soc. Jpn. 81, 104713 (2012)
- M. Ezawa, Euro. Phys. J. B 85, 363 (2012)
- M. Ezawa, Phys. Rev. B 86, 161407(R)

M. Ezawa, Phys. Rev. Lett 110, 026603 (2013)

9. "Hexagonally Warped Dirac Cones and Topological Phase Transition in Silicene Superstructure"

M. Ezawa, Euro. Phys. J. B 86, 139 (2013)

- 10. "Spin-Valleytronics in Silicene: Quantum-Spin-Quantum-Anomalous Hall Insulators and Single-Valley Semimetals"
  - M. Ezawa, Phys. Rev. B 87, 155415 (2013)
- 11. "Interference of Topologically Protected Edge States in Silicene Nanoribbons" M. Ezawa and N. Nagoasa, cond-mat/arXiv:1301.6337
   12. "Half-Integer Quantum Hall Effects in Silicene" M. Ezawa, cond-mat/arXiv:1302.2284
- 13. "Quantized Conductance and Field-Effect Topological Quantum Transistor in Silicene Nanoribbons"

M. Ezawa, Appl. Phys. Lett. 102, 172103 (2013)

14. "Charge Transport in a Silicene pn Junction" A. Yamakage, M. Ezawa, Y. Tanaka and N. Nagaosa, cond-mat/arXiv:1303.1245
15. "Quantum Hall Effects with High Spin-Chern Numbers in Buckled Honeycomb Structure with Magnetic Order" M. Ezawa, cond-mat/arXiv:1306.

## Review on silicene PHYSICS

#### ●内容の範囲

固体物理(結晶、アキルファス物質、金属物性, 速電体, 単環体, 副体 体, 光学的一熱的, 機械的性質 など) 固体物理の応用(半環体素 子, 磁性材料, 光学的高品材料, レーザー など) 実験法, 実験装置 (分析)計測機器, 自動化機器, 計算機 など) 固体物理周辺の最近 の話題 そのほか (処理, 内外ニュース, 書籍の紹介 など)

### 固体物理

2013年4月·第48巻第4号

解説アー	モルファスシリコンにおける拡張指数関数型緩和現象 	
実験室 1	00テスラ超強磁場の高精度磁化測定	
トピックス	グラフェンからシリセンへ:シリコンでできたトポロジカル絶縁体 	
トピックス	マルチフェロイックス物質中の磁気スキルミオン 関真一郎・于秀珍・石渡晋太郎・十倉好紀・41(179)	_ (
サロン 牧	9性/素粒子の学際を学部生と楽しめるか	F

#### トピックス

グラフェンからシリセンへ: シリコンでできたトポロジカル絶縁体

東京大学大学院工学系研究科 江澤雅彦

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#### Review

Relaxation Phenomena of Stretched Exponential Function Type in Amorphous Silicon by Kazuo Morigaki, Harumi Hikita, and Kosei Takeda · 1 (139) Relaxation phenomena characterized by stretched exponential function as their relaxation function in amorphous silicon are reviewed, taking the following phenomena: Light-induced defect creation, light-induced electron spin resonance, and photoluminescence in hydrogenated amorphous silicon.

#### Laboratory Guide

Precise Magnetization Measurement in Magnetic Fields above 100 T

by Shojiro Takeyama  $\cdot$  13 (151) We developed a precision magnetization measurement system used in the vertical-type single-turn coil ultra-high magnetic field generator. A low-temperature cryogenic container was specialy designed for this system and acomplished. The measurement system was applied to reveal magnetization processes in frustrated chromium spinel CdCr<sub>2</sub>O<sub>4</sub>.

#### Topics

From Graphene to Silicene: Silicon-based Topological Insulators

by Motohiko Ezawa 23 (161) Silicene is a monolayer of silicon atoms forming a two-dimensional honeycomb lattice. The low energy theory is described by Dirac electrons as in graphene, but they are massive due to spin-orbit interaction. Remarkably the band gap of silicene can be controlled externally by tuning electric field, photo-irradiation and antiferromagnetic order. Silicene shows a rich variety of topological insulators such as a quantum spin-Hall insulator, a quantum anomalous-Hall insulator and a hybrid of them. It also yields a topological semimetal such as a single Dirac-cone state where the half-integer quantum Hall effect will be realized. The band gap can be measured by way of optical absorption and orbital diamagnetism.

#### Topics

Observation of Skyrmions in a Multiferroic Material

by Shinichiro Seki, Xiuzhen Yu, Shintaro Ishiwata, and Yoshinori Tokura · 41 (179) We report the experimental discovery of skyrmions (nanometer-scale vortex-like spin texture) in an insulating chiral-lattice magnet Cu<sub>2</sub>OSeO<sub>2</sub>. Skyrmions in insulator can magnetically induce electric polarization through the relativistic spin-orbit interaction, which may potentially enable the manipulation of the skyrmion by an external electric field without losses due to joude heating.

#### Salon

Can we enjoy interdisciplinary regime between condensed matter physics and high energy physics with undergraduate students?

#### by Hideo Aoki · 55 (193)

A description is given of an attempt at having a seminar on interdisciplinary topics encompassing the two branches of physics in an undergraduate class in the University of Tokyo.

## **ARPES** of Silicene

a) K<sup>s</sup> 1 nm a)  $E_{F} = 0 -$ -1.0--2.0b) -3.0----0.8  $k_{\parallel}(A^{-1})$ Si on-top of a Ag atom Si between Ag atoms c) Ag atom

Guy Le Lay et al, Phys. Rev. Lett. 108, 155501 (2012)



Presence of gapped silicene-derived band in the prototypical (3x3) silicene phase on silver (111) surfaces



# STM and LEED Experiments

### Low-energy electron diffraction





N. Takagi, M. Kawai et.al., Appl. Phys. Express 5, 045802 (2012).







## Silicene on Ir(111)



## Experiment on Bilayer Silicene



### C Si Ge Sn A Graphene, silicene, germanene, tinene?

Silicene and Germanene

Spin orbit interactions become drastically larger as increasing atomic number

	t(eV)	$v_{\rm F}(10^{5}{\rm m/s})$	<i>a</i> (Å)	$\lambda_{SO}(meV)$	$\lambda_{R2}$	$\ell$	θ
Graphene	2.8	9.8	2.46	$10^{-3}$	0	0	90
Silicene	1.6	5.5	3.86	3.9	0.7	0.23	101.7
Germanene	1.3	4.6	4.02	43	10.7	0.33	106.5

Fermi velocity smaller

C-C, Liu, H.Jiang and Y. Yao, PRB 84 195430 (2011)



Tight Binding ModelSpin-orbit term
$$t = 1.6 \text{ eV}$$
 $H = -t \sum_{\langle i,j \rangle \alpha} c_{i\alpha}^{\dagger} c_{j\alpha} + i \frac{\lambda_{SO}}{3\sqrt{3}} \sum_{\langle \langle i,j \rangle \rangle \alpha \beta} v_{ij} c_{i\alpha}^{\dagger} \sigma_{\alpha\beta}^{z} c_{j\beta}$  $\lambda_{SO} = 3.9 \text{ meV}$  $H = -t \sum_{\langle i,j \rangle \alpha} c_{i\alpha}^{\dagger} c_{j\alpha} + i \frac{\lambda_{SO}}{3\sqrt{3}} \sum_{\langle \langle i,j \rangle \rangle \alpha \beta} v_{ij} c_{i\alpha}^{\dagger} \sigma_{\alpha\beta}^{z} c_{j\beta}$  $\lambda_{SO} = 3.9 \text{ meV}$  $\lambda_{R} = 0.7 \text{ meV}$  $\lambda_{R} = 0.7 \text{ meV}$  $-i \frac{2}{3} \lambda_{R2} \sum_{\langle \langle i,j \rangle \rangle \alpha \beta} \mu_{i} c_{i\alpha}^{\dagger} \left( \sigma \times \hat{d}_{ij} \right)_{\alpha\beta}^{z} c_{j\beta} c_{j\beta}$  $l = 0.23 \text{ Å}$ + controllable interactions

C. L. Kane and E. J. Mele, PRL 95. 226801 (2005) C-C, Liu, H.Jiang and Y. Yao PRB **84** 195430 (2011)

M. Ezawa, NJP 14 033003 (2012); PRL 109, 055502 (2012); PRL 110, 026603 (2013); PRB 87, 155415 (2013)



Dirac Theory of Silicene

• Low-energy dynamics of silicene is described by the Dirac theory as in graphene:

$$H_{\eta} = \hbar v_{\rm F} \left( \eta k_x \tau_x + k_y \tau_y \right) + \eta \tau_z \lambda_{\rm SO} \sigma_z$$
$$+ \eta \tau_z a \lambda_{\rm R2} \left( k_y \sigma_x - k_x \sigma_y \right)$$
$$+ \text{ controllable interactions}$$

- Possible interactions are of the form:  $H_{pqr} = \lambda_{pqr} \eta^p (\sigma_z)^q (\tau_z)^r$
- The Dirac mass:

$$v_{\rm F} = \frac{\sqrt{3}}{2}at = 5.5 \times 10^5 {\rm m/s}$$

- $\lambda_{111} = \lambda_{SO}$
- $\lambda_{001} = -\ell E_z$

 $\lambda_{011} = \Delta M$ 

Electric field

SO interaction

- $\lambda_{101} = \lambda_{\Omega}$  Photo-irradiation
  - Exchange fields

14

$$\Delta_{s_z}^{\eta} = \eta s_z \lambda_{\rm SO} - \ell E_z + \eta \lambda_{\Omega} + s_z \Delta M$$

M. Ezawa, NJP 14 033003 (2012); PRL 109, 055502 (2012); PRL 110, 026603 (2013); PRB 87, 155415 (2013)

## Tight Binding Model (2)



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 $H = -t \sum_{\langle i,j \rangle \alpha} c^{\dagger}_{i\alpha} c_{j\alpha} + i \frac{\lambda_{\rm SO}}{3\sqrt{3}} \sum_{\langle \langle i,j \rangle \rangle \alpha\beta} v_{ij} c^{\dagger}_{i\alpha} \sigma^{z}_{\alpha\beta} c_{j\beta}$ Spin-orbit term  $-i\frac{2}{3}\lambda_{R2} \sum \mu_i c^{\dagger}_{i\alpha} \left(\boldsymbol{\sigma} \times \hat{\boldsymbol{d}}_{ij}\right)^z_{\alpha\beta} c_{j\beta}$ Second Rashba term  $\langle\!\langle i,j \rangle\!\rangle \alpha \beta$ **Electric field**  $-\ell \sum_{i\alpha} t_z^i E_z c_{i\alpha}^{\dagger} c_{i\alpha} + i \frac{\lambda_{\Omega}}{3\sqrt{3}} \sum_{\langle\!\langle i,j \rangle\!\rangle \alpha\beta} \nu_{ij} c_{i\alpha}^{\dagger} c_{j\beta}$ Photo-irradiation Exchange field  $+\sum M_{t_z^i} c_{i\alpha}^{\dagger} \sigma_z c_{i\alpha} \implies \Delta M \sigma_z \tau_z + \overline{M} \sigma$  $\overline{M} = (M_A + M_B)/2,$  $i\alpha$  $\Delta M = (M_A - M_B)/2$ 

M. Ezawa, NJP 14 033003 (2012); PRL 109, 055502 (2012); PRL 110, 026603 (2013); PRB 87, 155415 (2013)

## Controllable Gap of Silicene

• The simplest example with the use of the electric field  $E_z$ 



M.Ezawa, NJP 14 033003 (2012)

## Bulk-Edge Correspondence

### Bulk-edge correspondence gives

#### an excellent signal of a topological insulator



- Gapless edge modes emerge along the phase boundary between two different topological insulators
- They are topologically protected
- Each gapless mode provides one conduction channel along the edge





### Emergence of Edge Modes in Armchair Edge



## Quasiparticle interference

16

8

6

x (nm)





2

x (nm)



armchair



B. Feng, K. Wu et al. cond-mat/arXiv:1304.3308

6 x (nm)

2 4

10

2

## DOS and Quantized Conductance



- Easiest way to observe the topological phase transition
- One quantized conductance per one channel
- Unit conductance is  $e^2/h$
- Conductance is different in each phase
- Field-effect topological quantum transistor

<u> </u>	topological insulator	QAH	QSH	SQAH	trivial
	topological numbers	(2,0)	(0,1)	(1, 1/2)	(0,0)
ר	conductance $(\sigma)$	2	2	1	0

## **Topological Phase Transition**

- Topological phase transition occurs when the sign of Dirac mass changes
- Dirac mass in silicene is given by

$$\Delta_{s_z}^{\eta} = \eta s_z \lambda_{\rm SO} - \ell E_z + \eta \lambda_{\Omega} + s_z \Delta M$$

- Electric field induced mass term
- Photo-induced Haldane mass term
- Antiferromagnet-induced mass term

	Order	TRS	SRS	SLS
111	Kane-Mele	True	False	False
001	CDW	True	True	False
011	AF	False	False	False
101	Haldane	False	True	False

## Chern and Spin Chern Numbers

- A Spin Chern number(Mod2) =  $Z_2$  index, when  $s_z$  is conserved
- A They are determined by the Dirac mass

$$C_{s_{z}}^{\eta} = \frac{1}{4\pi} \int d^{2}k \left( \frac{\partial \hat{\mathbf{d}}}{\partial k_{x}} \times \frac{\partial \hat{\mathbf{d}}}{\partial k_{y}} \right) \cdot \hat{\mathbf{d}} \quad \qquad \text{Pontryagin number}$$

$$C_{s_{z}}^{\eta} = \frac{\eta}{4\pi} \int d^{2}k \, \varepsilon_{ij} \partial_{i} \sigma \partial_{j} \theta = \frac{\eta}{2} \int_{0}^{1} d\sigma = \frac{\eta}{2} \operatorname{sgn}(\Delta_{s_{z}}^{\eta}) \quad \sigma(k) = \frac{\Delta_{s_{z}}^{\eta}}{\sqrt{(\hbar v_{\mathrm{F}} k)^{2} + (\Delta_{s_{z}}^{\eta})^{2}}}$$

$$H_{\eta} = \left( \begin{array}{c} \Delta_{s_{z}}^{\eta} & \hbar v_{\mathrm{F}}(\eta k_{x} - ik_{y}) \\ \hbar v_{\mathrm{F}}(\eta k_{x} + ik_{y}) & -\Delta_{s_{z}}^{\eta} \end{array} \right)$$

$$H = \tau \cdot \mathbf{d}$$

$$d_{x} = \eta \hbar v_{\mathrm{F}} k_{x}, \quad d_{y} = \hbar v_{\mathrm{F}} k_{y}, \quad d_{z} = \Delta_{s_{z}}^{\eta}$$
Meron pseudospin texture

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M.Ezawa, Euro. Phys. J. B 85, 363 (2012)

### Classification of Topological Insulators

$\mathcal{C}^K_\uparrow$	$\mathcal{C}^{K'}_{\uparrow}$	$\mathcal{C}^K_\downarrow$	$\mathcal{C}^{K'}_{\downarrow}$	$\mathcal{C}$	$2\mathcal{C}_s$	$\mathcal{C}_v$	$\mathcal{C}_{sv}$	
1/2	1/2	1/2	1/2	2	0	0	0	QAH
1/2	1/2	1/2	-1/2	1	1	1	-1	SQAH
1/2	1/2	-1/2	1/2	1	-1	1	1	SQAH
1/2	1/2	-1/2	-1/2	0	0	2	0	CDW
1/2	-1/2	1/2	1/2	1	1	-1	1	SQAH
1/2	-1/2	1/2	-1/2	0	2	0	0	QSH
1/2	-1/2	-1/2	1/2	0	0	0	2	AF
1/2	-1/2	-1/2	-1/2	-1	1	1	1	SQAH
-1/2	1/2	1/2	1/2	1	-1	-1	-1	SQAH
-1/2	1/2	1/2	-1/2	0	0	0	-2	AF
-1/2	1/2	-1/2	1/2	0	-2	0	0	QSH
-1/2	1/2	-1/2	-1/2	-1	-1	1	-1	SQAH
-1/2	-1/2	1/2	1/2	0	0	-2	0	CDW
-1/2	-1/2	1/2	-1/2	-1	1	-1	-1	SQAH
-1/2	-1/2	-1/2	1/2	-1	-1	-1	1	SQAH
-1/2	-1/2	-1/2	-1/2	-2	0	0	0	QAH

Chern number

$$\mathcal{C} = \mathcal{C}^K_{\uparrow} + \mathcal{C}^{K'}_{\uparrow} + \mathcal{C}^K_{\downarrow} + \mathcal{C}^{K'}_{\downarrow}$$

Spin-Chern number

$$\mathcal{C}_s = \frac{1}{2} (\mathcal{C}^K_{\uparrow} + \mathcal{C}^{K'}_{\uparrow} - \mathcal{C}^K_{\downarrow} - \mathcal{C}^{K'}_{\downarrow})$$

Valley-Chern number

$$\mathcal{C}_{v} = (\mathcal{C}_{\uparrow}^{K} - \mathcal{C}_{\uparrow}^{K'} + \mathcal{C}_{\downarrow}^{K} - \mathcal{C}_{\downarrow}^{K'})$$

Spin-Valley Chern number

$$\mathcal{C}_{sv} = \frac{1}{2} (\mathcal{C}^K_{\uparrow} - \mathcal{C}^{K'}_{\uparrow} - \mathcal{C}^K_{\downarrow} + \mathcal{C}^{K'}_{\downarrow})$$

F. Zhang, J. Jung, G.A. Fiete, Q. Niu, and A.H. MacDonald PRL 106, 156801 (2011)

M. Ezawa, Phys. Rev. B 87, 155415 (2013)

## Silicene with Exchange Interaction



 $i\alpha$ 



M. Ezawa, PRL 109, 055502 (2012)

W.K. Tse Z. Qiao, Y. Yao, A. H. MacDonald, and Qian Niu, PRB 83, (2011) 155447.

## Quantum Anomalous Hall Effect

- QAHE is QHE without magnetic field (nonzero Chern number)
- The QAH phase has flat gapless edge modes



Without Rashba interaction M. Ezawa, PRL 109, 055502 (2012)



With Rashba interaction





## Valley Polarized Metal

### Valley polarization



#### M. Ezawa, PRL 109, 055502 (2012)



### Antiferromagnet and Electric Fields





M. Ezawa, PRB 87, 155415 (2013)

## QHE with High Spin-Chern Number





### Photo-Induced Topological Phase Transition



#### Topological Semimetal and Topological Metal

- Two types of topological phase transitions
- One occurs when the Dirac mass becomes zero, (electric field, photo-irradiation, antiferromagnet)

 $\Delta_{s_z}^{\eta} = \eta s_z \lambda_{\rm SO} - \ell E_z + \eta \lambda_{\Omega} + s_z \Delta M.$ 

- Other occurs when the band edge touches the Fermi energy (ferromagnet)
- Provided it is sandwiched by two different topological insulators, a topological semimetal or metal emerge along the phase boundary





## Conclusion



- Silicene is a graphene-like silicon honeycome structure
- The band gap can be tuned by external electric field
- Topologically protected zero-energy edge channels transport quantized conductance topological quantum nanodevices
- Many new topological phases emerge in silicen
- **CALE** with flat chiral edge and momentum skyrmion
- **★***QAHE* with anisotropic chiral edge
- ★ Single Dirac Cone State, ★ Spin-Polarized QHE
- **+** Hybrid Topological Insulator, **+** Single-Valley Semimetal
- **★** Topological Semimetal and Topological Metal

### Quantum Anomalous Hall Effects in Graphene

#### QAH is QH without magnetic field (nonzero Chern number)



Z. Qiao, S. A. Yang, W. Feng, W.-K. Tse, J. Ding, Y. Yao, J. Wang, and Q. Niu PRB 82, 161414R (2010)
W.-K. Tse, Z. Qiao, Y. Yao, A. H. MacDonald, and Q. Niu, PRB 83, 155447 (2011)
Z. Qiao, H. Jiang, X. Li, Y. Yao, and Q. Niu, PRB 85, 115439 (2012)
M. Ezawa, PRL 109, 055502 (2012); PRL110, 026603 (2013)



## Various Superstructures

Ag 145 pm Si 111 pm 145/111=1.31



$$\tan \phi = \sqrt{3}q/(2p+q)$$
$$|g_1| = \sqrt{p^2 + q^2 + pq}$$
$$N = 2|g_1|^2 = 2(p^2 + q^2 + pq)$$

M. Ezawa, Euro. Phys. J. B 86, 139 (2013)

Ag-superstructure	Si-superstructure	p	q	ratio
$4 \times 4[1, 2]$	$3 \times 3$	3	0	1.33
$\sqrt{7} \times \sqrt{7}$	$2 \times 2$	2	0	1.32
$\sqrt{13} \times \sqrt{13}$ [2]	$\sqrt{7}  imes \sqrt{7}$	2	1	1.36
$\sqrt{21} \times \sqrt{21}$	$2\sqrt{3} \times 2\sqrt{3}$	2	2	1.32
$2\sqrt{3} \times 2\sqrt{3}$ [17]	$\sqrt{7}  imes \sqrt{7}$	2	1	1.31
(free-standing)	$1 \times 1$	1	0	
nothing	$\sqrt{3} \times \sqrt{3}$	1	1	

$$egin{aligned} m{g}_1 &= p m{a}_1 + q m{a}_2 \ m{g}_2 &= e^{\pm i \pi/3} m{g}_1 \ m{K} - m{K}' &= n_1 m{G}_1 + n_2 m{G}_2 \ m{G}_i &= (m{g}_i imes m{n}) / |m{g}_1 imes m{g}_2| \end{aligned}$$

#### Topological Insulator, Semimetal and Metal



## Chern and Spin Chern Numbers

- A Spin Chern number(Mod2) =  $Z_2$  index, when  $s_z$  is conserved
- A They are determined by the Dirac mass

$$C_{s_{z}}^{\eta} = \frac{1}{4\pi} \int d^{2}k \left( \frac{\partial \hat{\mathbf{d}}}{\partial k_{x}} \times \frac{\partial \hat{\mathbf{d}}}{\partial k_{y}} \right) \cdot \hat{\mathbf{d}} \quad \qquad \text{Pontryagin number}$$

$$C_{s_{z}}^{\eta} = \frac{\eta}{4\pi} \int d^{2}k \, \varepsilon_{ij} \partial_{i} \sigma \partial_{j} \theta = \frac{\eta}{2} \int_{0}^{1} d\sigma = \frac{\eta}{2} \operatorname{sgn}(\Delta_{s_{z}}^{\eta}) \quad \sigma(k) = \frac{\Delta_{s_{z}}^{\eta}}{\sqrt{(\hbar v_{\mathrm{F}} k)^{2} + (\Delta_{s_{z}}^{\eta})^{2}}}$$

$$H_{\eta} = \left( \begin{array}{c} \Delta_{s_{z}}^{\eta} & \hbar v_{\mathrm{F}}(\eta k_{x} - ik_{y}) \\ \hbar v_{\mathrm{F}}(\eta k_{x} + ik_{y}) & -\Delta_{s_{z}}^{\eta} \end{array} \right)$$

$$H = \tau \cdot \mathbf{d}$$

$$d_{x} = \eta \hbar v_{\mathrm{F}} k_{x}, \quad d_{y} = \hbar v_{\mathrm{F}} k_{y}, \quad d_{z} = \Delta_{s_{z}}^{\eta}$$
Meron pseudospin texture

M.Ezawa, Euro. Phys. J. B 85, 363 (2012)

## Honeycomb AF-Dirac System

Monolayer antiferromagnetic manganese chalcogenophosphates (MnPX3, X = S, Se) Xiao Li, Ting Cao, Qian Niu, Junren Shi, Ji Feng, cond-mat/arXiv:1210.4623

perovskite G-type antiferromagnetic insulators grown along [111] direction Qi-Feng Liang, Long-Hua Wu, Xiao Hu, cond-mat/arXiv:1301.4113



## Floquet Perturbation Theory

- ▲ Effective Hamiltonian  $\Delta H_{\text{eff}} = (i\hbar/T)\log U$
- Time evolution operator  $U = \mathcal{T} \exp[-i/\hbar \int_0^T H(t) dt]$
- Second order  $\Delta H_{\text{eff}} = (\hbar \Omega)^{-1} [H_{-1}, H_{+1}] + O(\mathcal{A}^4)$
- Floquet component  $H_{\pm 1} = \frac{1}{T} \int_0^T H(T) e^{\pm it |\Omega|} dt$  $\Delta H_{\rm eff} = -\frac{\mathcal{A}^2}{\hbar \Omega} \left[ \left( \hbar v_{\rm F} \right)^2 \eta \tau_z \right]$
- Haldane interaction
- Haldane term  $\Delta H_{\text{eff}} = i\eta \hbar v_{\text{F}}^2 \mathcal{A}^2 / (3\sqrt{3}\Omega) \sum \nu_{ij} c_{i\alpha}^{\dagger} c_{j\beta}$

 $\langle \langle i, j \rangle \rangle \alpha \beta$  Dirac mass  $m_{\rm D} = -s_z t_z \lambda_{\rm SO} + \ell E_z - \eta \hbar v_{\rm F}^2 \mathcal{A}^2 \Omega^{-1}$ T. Kitagawa, T. Oka, A. Brataas, L. Fu, and E. Demler, Phys. Rev.B 84, 235108 (2011). 42

## **Optical Absorption of Silicene**



photo-induced transition from the valence band to the conduction band at the K point

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

Electromagnetic potential  $A(t) = (A \sin \omega t, A \cos \omega t)$ Covariant momentum  $P_i \equiv \hbar k_i + eA_i$ 

 $H_{\xi}(A) = H_{\xi} + \mathcal{P}_{x}^{\xi}A_{x} + \mathcal{P}_{y}^{\xi}A_{y}$ 

Circular polarization

$$\begin{aligned} \mathcal{P}_x^{\xi} &= \frac{1}{\hbar} \frac{\partial H_{\xi}}{\partial k_x} = v_{\mathrm{F}} \xi \tau_x - \frac{a \lambda_{\mathrm{R2}}}{\hbar} \xi \tau_z \sigma_y, \\ \mathcal{P}_y^{\xi} &= \frac{1}{\hbar} \frac{\partial H_{\xi}}{\partial k_y} = v_{\mathrm{F}} \tau_y + \frac{a \lambda_{\mathrm{R2}}}{\hbar} \xi \tau_z \sigma_x, \end{aligned}$$

## Silicene (monolayer honeycomb-silicon)

- Experimentally manufactured in 2012 (last year)
- Striking properties similar to graphene
   but more ramakable than graphene
- A The low energy structure is described by Dirac fermions
- Buckled structure owing to a large ionic radius of silicon
- Relatively large spin-orbit gap of 3.9meV
- A The band gap is controllable by applying the electric field
- A The gap closes at a certain critical electric field
- A Almost all topological phases can be materialized
- ▲ QHE, QSHE, QAHE, P-QHE(no LL), .....

## Skymions



 Skyrmions are solitons in a nonlinear field theory characterized by the topological quantum number

 $S^2 \to S^2$ 

 $S^2$ 

compactification

 $S^2$ 

**φ**(x)

mapping

- Skyrmion is a nontrivial spin texture in 2D<sup>№</sup>
- Homotopy class

$$\pi_2\left(S^2\right) = \mathbb{Z}$$

Non zero Pontryagin number

$$Q_{\rm sky} = -\frac{1}{8\pi} \sum_{ij} \int d^2 x \varepsilon_{ij} \boldsymbol{n}(\boldsymbol{x}) \cdot (\partial_i \boldsymbol{n}(\boldsymbol{x}) \times \partial_j \boldsymbol{n}(\boldsymbol{x}))$$

## 3x3 Si-Superstructure

#### K and K' points become identical

G2\/G1





M.Ezawa, cond-mat/arXiv:1209.2580



## Silicon Nanotube & Carbon Nanotube

#### Silicon nanotube is constructed by rolling up a silicene



#### J. Sha, et.al., Advanced Materials,

14 1219 (2002)





De Crescenzi et al. Appl. Phys. Lett. **86**, 231901 (2005)

M.Ezawa, Europhysics Letters 98, 67001 (2012)

# Coupling the valley degree of freedom to antiferromagnetic order



X. Li, T. Cao, Q. Niu, J. Shi, and J. Feng, cond-mat/arXiv:1210.4623

## Inhomogeneous Electric Field

We apply the electric field  $E_z(x)$  perpendicularly to a silicene sheet homogeneously in the *y*-direction and inhomogeneously in the *x*-direction.

A Helical Jackiw–Rebbi mode  $\Psi(x, y) = e^{ik_y y} \Phi(x) \quad \phi_B(x) = i\xi \phi_A(x)$ 

$$H_{\eta}\phi_A(x) = E_{\eta\xi}\phi_A(x) \quad E_{\eta\xi} = \eta\xi\hbar v_{\rm F}k_y$$

Equation of motion  $(\xi \hbar v_{\rm F} \partial_x + \eta \lambda_{\rm SO} \sigma_z - \ell E_z(x)) \phi_A(x) = 0.$ 

A Localized state  $f(x) = C \exp\left[\frac{\xi}{\hbar v_{\rm F}} \int^{x} (-\eta s_z \lambda_{\rm SO} + \ell E_z(x')) \, \mathrm{d}x'\right]$   $J_{s_z}(x) = \operatorname{Re}\left[\frac{\hbar}{2mi} \Psi_{s_z}^{\dagger} \partial_y \Psi_{s_z}\right] = \frac{\hbar k_y}{m} |\phi_{\rm As_z}(x)|^2$ 

M.Ezawa, NJP 14 033003 (2012)



## Perpendicular Electric Field

• Effective electric field is given by  $E_z(x) = E \sin \theta_{\rm B}$ 





 $\theta_2 \quad \theta_3$ 

The wave function of each zero mode is

localized within the metallic region

0.10

**1**0

 $E_{Z} = \begin{bmatrix} \theta_{2} \\ \\ \theta_{3} \end{bmatrix}$ 

There emerge four helical zero modes propagating along the nanotube

M.Ezawa, Europhysics Letters 98, 67001 (2012)

L

Various Superstructures

$$g_1 = pa_1 + qa_2, \qquad g_2 = e^{\pm \pi/3}g_1$$

Ag 145 pm Si 111 pm 145/111=1.31

$$N = 2 |\mathbf{g}_1|^2 = 2 (p^2 + q^2 + pq)$$
  
$$\tan \phi = \sqrt{3}q/(2p+q)$$

 $|g_1| = \sqrt{p^2 + q^2 + pq}$ 

Ag-superstructure	Si-superstructure	p	q	ratio
$4 \times 4[1, 2]$	$3 \times 3$	3	0	1.33
$\sqrt{7} \times \sqrt{7}$	$2 \times 2$	2	0	1.32
$\sqrt{13} \times \sqrt{13}$ [2]	$\sqrt{7}  imes \sqrt{7}$	2	1	1.36
$\sqrt{21} \times \sqrt{21}$	$2\sqrt{3} \times 2\sqrt{3}$	2	2	1.32
$2\sqrt{3} \times 2\sqrt{3}$ [17]	$\sqrt{7}  imes \sqrt{7}$	2	1	1.31
(free-standing)	$1 \times 1$	1	0	
nothing	$\sqrt{3} \times \sqrt{3}$	1	1	

$$\boldsymbol{K} - \boldsymbol{K}' = n_1 \boldsymbol{G}_1 + n_2 \boldsymbol{G}_2$$

 $m{G}_1 = (m{g}_2 imes m{n}) / |m{g}_1 imes m{g}_2|$ , M.Ezawa, cond-mat/arXiv:1209.2580

$$G_2 = (\boldsymbol{g}_1 \times \boldsymbol{n}) / |\boldsymbol{g}_1 \times \boldsymbol{g}_2|,$$



FIG. 3: (Color online) Band structure of silicene at the critical electric field  $E_c$ . (a) A bird's-eye view. Dirac cones are found at 6 corners of the hexagonal Brillouin zone. (b) The cross section containing a pair of K and K' points. The solid red (dashed blue) band is for up-spin (down-spin) electrons, which are gapless (gapped) at the K point but gapped (gapless) at the K' point.

M.Ezawa, NJP 14 033003 (2012)

## Band Structure of Silicene Nanoribbon

1.0







## **Topological Insulator**

- Topology charge is defined for an insulator
- Topological insulator has a nontrivial topological charge
- Surface has a gapless modes
- *Chiral* or *Helical* edge modes
- Quantum Spin Hall effects helical edge
- QAH effects



## Bulk-Edge Correspondence

- If a bulk has a non-trivial topological number, the edge has gapless edge modes due to the discontinuity of the topological number.



topological insulator





## Chern Number and Meron

- ▲ SU(2) Hamiltonian  $H = \tau \cdot d$
- Chern number
- Pontryagin number

$$\mathcal{C} = \frac{1}{4\pi} \int d^2k \left( \frac{\partial \hat{d}}{\partial k_x} \times \frac{\partial \hat{d}}{\partial k_y} \right) \cdot \hat{d}$$

A Chern number is determined by the sign of Dirac mass

$$H = \begin{pmatrix} m_{\rm D} & \hbar v_{\rm F} \left( k_x + i k_y \right) \\ \hbar v_{\rm F} \left( k_x - i k_y \right) & -m_{\rm D} \end{pmatrix}$$
$$\mathcal{C}_{s_z}^{\eta} = \frac{\eta}{2} \mathrm{sgn} \left( m_{\rm D} \right)$$

- Meron in momentum space
- Meron is a topological object with a half Pontyragin number

## Phase Diagram in E-M plane

- Quantum spin Hall (QSH)
- Quantum anomalous Hall
- Valley polarized metal (VPM)
- Marginal-VPM
- Spin-Valley polarized metal
- Band insulator (BI)



FIG. 1: (Color online) Phase diagram in the  $E_z$ -M plane. Dotted lines represent the points where the band gap closes. Heavy lines represent phase boundaries. A circle shows a point where the energy spectrum is calculated and shown in Fig.2.

M.Ezawa, cond-mat/arXiv:1203.0705 (to be publisehd in PRL)

## Silicon Nanotube from Silicene

- Chiral vector  $\mathbf{L} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$
- A Nanotube circumference  $L = |\mathbf{L}| = a\sqrt{n_1^2 + n_2^2 - n_1 n_2}$
- A Periodic boundary condition  $\psi(x + L, y) = \psi(x, y)$
- A Descretization of k<sub>x</sub>  $k_x = 2\pi j/L$   $j = 0, 1, \dots, 2n - 1$
- A Brilloin zone  $-\pi/T \le k_y \le \pi/T$
- Energy spectrum of silicon nanotube  $E_j(k_y) = \mathcal{E}(k_x, k_y)$





Fig. 5: (Color online) An illustration of silicon nanotube under electric field  $E > E_{\rm cr}$ . There appear two topological insulator regions and two band insulator regions. They are separated by metallic states made of helical zero modes. A spin current flows in each metallic region as indicated. For instance, up-spin (down-spin) electrons propagate into the left (right) direction at  $\theta = \theta_1$ .

M.Ezawa, Europhysics Letters 98, 67001 (2012)

### Silicon Nanotube vs Silicene Nanoribbon



## Quantum Hall Effects in Silicene

$$\hat{a} = \frac{\ell_B (P_x + iP_y)}{\sqrt{2\hbar}}, \quad \hat{a}^{\dagger} = \frac{\ell_B (P_x - iP_y)}{\sqrt{2\hbar}}$$
$$\begin{pmatrix} \Delta_+ (E_z) & \hbar \omega_c \hat{a} & i\frac{\sqrt{2\hbar a\lambda_R}}{\ell_B} \hat{a}^{\dagger} & 0\\ \hbar \omega_c \hat{a}^{\dagger} & -\Delta_+ (E_z) & 0 & -i\frac{\sqrt{2\hbar a\lambda_R}}{\ell_B} \hat{a}^{\dagger}\\ -i\frac{\sqrt{2\hbar a\lambda_R}}{\ell_B} \hat{a} & 0 & \Delta_- (E_z) & \hbar \omega_c \hat{a}\\ 0 & i\frac{\sqrt{2\hbar a\lambda_R}}{\ell_B} \hat{a} & \hbar \omega_c \hat{a}^{\dagger} & -\Delta_- (E_z) \end{pmatrix}$$

$$\Psi_{+}^{N} = \left(u_{A\uparrow}^{N} |N\rangle, u_{B\uparrow}^{N+1} |N+1\rangle, u_{A\downarrow}^{N-1} |N-1\rangle, u_{B\downarrow}^{N} |N\rangle\right)^{t}$$

M.Ezawa, J. Phys. Soc. Jpn. 81, 064705 (2012)

## Quantum Hall effects in Silicene

4-fold degenerate zero-energy states are completely resolved even ٩ without considering Coulomb interactions.



M.Ezawa, J. Phys. Soc. Jpn. 81, 064705 (2012)

## Supersymmetric structure



M.Ezawa, cond-mat/arXiv:1202.1357

N=3

N=2

N=1

## Supersymmetric structure

$$\begin{aligned} H_{\eta}^{s_{z}} &= \hbar \omega_{c} Q_{\eta s_{z}} + \tau_{3} \Delta_{\eta s_{z}} \\ Q_{+} &= \begin{pmatrix} 0 & \hat{a} \\ \hat{a}^{\dagger} & 0 \end{pmatrix}, \quad Q_{-} &= \begin{pmatrix} 0 & \hat{a}^{\dagger} \\ \hat{a} & 0 \end{pmatrix} \\ (H_{\eta}^{s_{z}})^{2} &= (\hbar \omega_{c})^{2} Q_{\eta s_{z}} Q_{\eta s_{z}} + \Delta_{\eta s_{z}}^{2} (E_{z}) \\ H_{P}^{+} &= \begin{pmatrix} \hat{a} \hat{a}^{\dagger} & 0 \\ 0 & \hat{a}^{\dagger} \hat{a} \end{pmatrix} \end{aligned}$$

M.Ezawa, cond-mat/arXiv:1202.1357

$$Q = \begin{pmatrix} 0 & 0 \\ \hat{a}^{\dagger} & 0 \end{pmatrix}, \qquad Q^{\dagger} = \begin{pmatrix} 0 & \hat{a} \\ 0 & 0 \end{pmatrix}$$
$$H_{P}^{+} = \{Q, Q^{\dagger}\}, \qquad [H_{\eta}^{+}, Q] = 0$$
$$H_{P}^{+} = \hat{a}^{\dagger}\hat{a} + \hat{c}^{\dagger}\hat{c} \qquad \hat{c} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad \hat{c}^{\dagger} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$
$$\hat{c}|0\}_{B} = 0, \qquad \hat{c}^{\dagger}|0\}_{B} = |0\}_{A}, \qquad \hat{c}|0\}_{A} = |0\}_{B}$$
$$N_{A} = \frac{1}{\sqrt{N!}}\hat{a}^{\dagger N}|0\}_{A} = \begin{pmatrix} |N\rangle \\ |N\rangle_{B} = \frac{1}{\sqrt{N!}}\hat{a}^{\dagger N}|0\}_{B} = \begin{pmatrix} 0 \\ |N\rangle \end{pmatrix}$$
M.EzaWa, cond-mat/arXiV:1202.1357

## Energy level





M.Ezawa, cond-mat/arXiv:1202.1357

$$\begin{aligned} & \text{Dirac Fermions on Zigzag Edge} \\ & v_{\text{F}} \begin{pmatrix} 0 & p_{x} - ip_{y} \\ p_{x} + ip_{y} & 0 \end{pmatrix} \begin{pmatrix} \phi_{\text{A}}^{\text{K}}(\mathbf{x}) \\ \phi_{\text{B}}^{\text{K}}(\mathbf{x}) \end{pmatrix} = E \begin{pmatrix} \phi_{\text{A}}^{\text{K}}(\mathbf{x}) \\ \phi_{\text{B}}^{\text{K}}(\mathbf{x}) \end{pmatrix} \\ & v_{\text{F}} \begin{pmatrix} 0 & -p_{x} - ip_{y} \\ -p_{x} + ip_{y} & 0 \end{pmatrix} \begin{pmatrix} \phi_{\text{A}}^{\text{K}'}(\mathbf{x}) \\ \phi_{\text{B}}^{\text{K}'}(\mathbf{x}) \end{pmatrix} = E \begin{pmatrix} \phi_{\text{A}}^{\text{K}'}(\mathbf{x}) \\ \phi_{\text{B}}^{\text{K}'}(\mathbf{x}) \end{pmatrix} \\ & p_{x} - ip_{y} = -2i\hbar\partial_{z}, \quad p_{x} + ip_{y} = -2i\hbar\partial_{z}* \end{aligned}$$
$$\begin{aligned} & \partial_{z}*\phi_{\text{A}}^{\text{K}}(\mathbf{x}) = i\frac{E}{2\hbar}\phi_{\text{B}}^{\text{K}}(\mathbf{x}), \quad \partial_{z}\phi_{\text{B}}^{\text{K}}(\mathbf{x}) = i\frac{E}{2\hbar}\phi_{\text{A}}^{\text{K}}(\mathbf{x}), \\ & \partial_{z}\phi_{\text{A}}^{\text{K}'}(\mathbf{x}) = -i\frac{E}{2\hbar}\phi_{\text{B}}^{\text{K}'}(\mathbf{x}), \quad \partial_{z*}\phi_{\text{B}}^{\text{K}'}(\mathbf{x}) = -i\frac{E}{2\hbar}\phi_{\text{A}}^{\text{K}'}(\mathbf{x}). \end{aligned}$$
Cauchy-Riemann eq

Wave functions are holomorphic or antiholomorphic for E=0