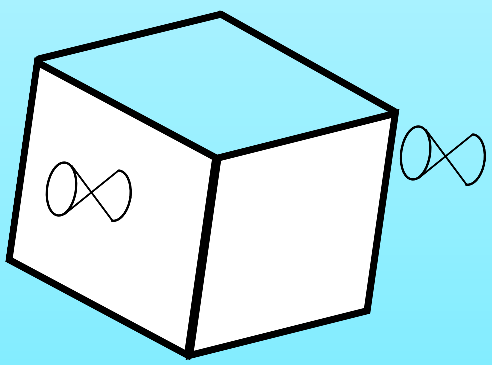
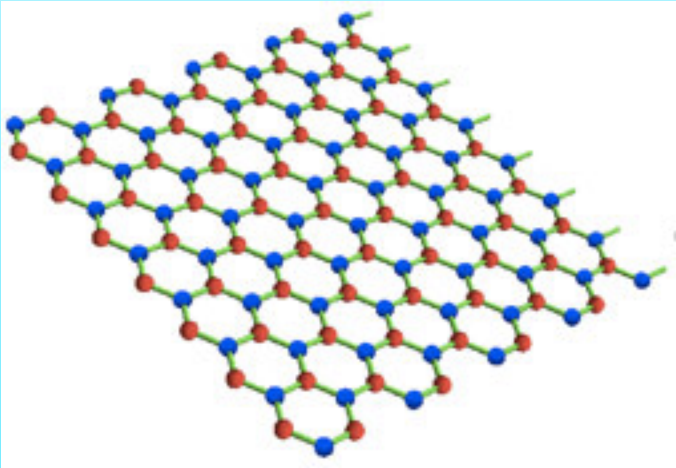
NWDTF12, March 9-10 Tohoku Univ. Sendai, 2013

Band gap, dangling bond & spin
A physicist's viewpoint

From Newton to Dirac



Institute of Physics, TIMS
University of Tsukuba
JAPAN
Yasuhiro Hatsugai



筑波大学・数理物質系・物理学域
初貝 安弘

東北大学
学際科学国際高等研究センター
Center for Interdisciplinary Research
Tohoku University

University of Tsukuba
筑波大学

The Nobel Prize in Physics 1956

William B. Shockley, John Bardeen, Walter H. Brattain

The Nobel Prize in Physics 1956

William B. Shockley

John Bardeen

Walter H. Brattain

William Bradford Shockley

John Bardeen

Walter Houser Brattain

The Nobel Prize in Physics 1956 was awarded jointly to William Bradford Shockley, John Bardeen and Walter Houser Brattain *"for their researches on semiconductors and their discovery of the transistor effect"*.

Plan

- ☆ Metal, insulator & semiconductor
- ☆ Bulk-edge correspondence :graphene, silicene and more
- ☆ From Newton to Dirac for devices breakthrough

Band inversion

Graphene & silisene

Edge states

Topological insulators

Spin-orbit int.

Massless Dirac fermions

Majorana fermions

Plan

- *Metal, insulator & semiconductor*
- *Bulk-edge correspondence :graphene, silicene and more*
- *From Newton to Dirac for devices breakthrough*

Metal, insulator & semiconductor

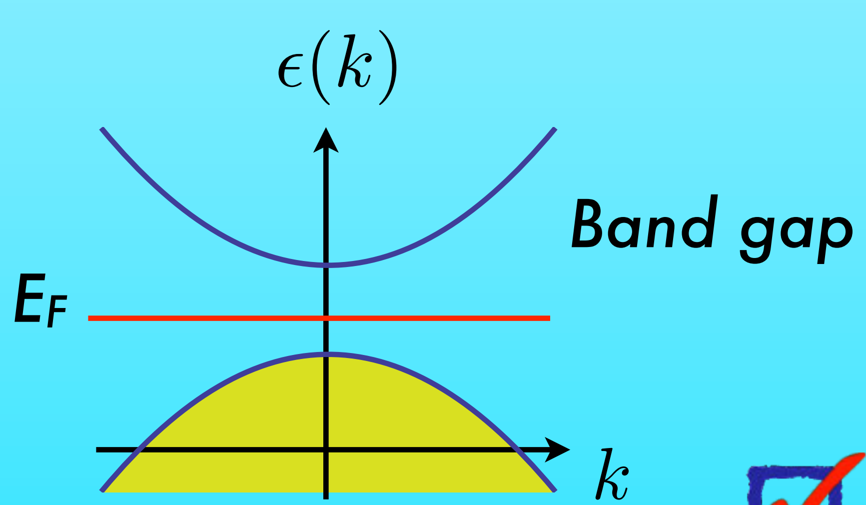
Metal & Semiconductor (doped)

? ? ?

??

打てども響かず

Insulator & Semiconductor (intrinsic)



- Useful !
  - carry current
- Interesting !
  - Response for small input
  - Lots of instabilities
    - magnetic ordering
    - superconductivity
    - ...

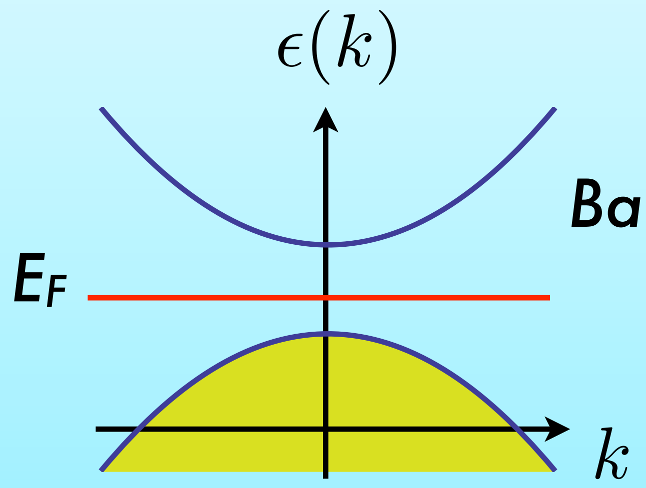
Q: Boring ?

Yes, maybe (before1980)

- No carrier
- No response for small perturbation

Metal, insulator & semiconductor

Insulator & Semiconductor (intrinsic)



Q: Boring ?

No, it's a fun (Today:2013)

- ☑ Useful !
  - Dissipationless current (?)
- ☑ Interesting !
  - Lots of varieties
    - Polarized phases
    - (Magneto-electric) polarization
    - With Spin-orbit with/without coulomb interaction

Non-trivial insulators (topological)

Metal, insulator & semiconductor

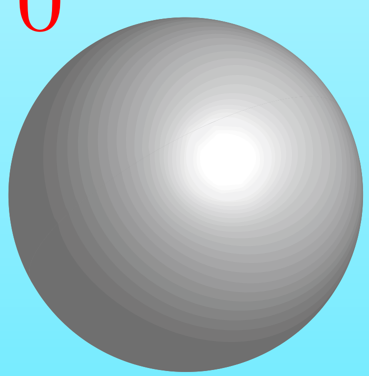
Topological $\approx$ Insulator (semiconductor)

Physics Stable for small but finite perturbation

math

g: # of holes

$g = 0$



$g = 1$

Metal, insulator & semiconductor

Topological ≈ Insulator (semiconductor)

Physics — Stable for small but finite perturbation

~~math~~ — Not joking: physicists are a bit more serious

Something

to be observed & useful !

"EDGE STATES"

"Dangling bonds" exist ! when non trivial !

Bulk-edge correspondence

Y. Hatsugai, Phys. Rev. Lett. 71, 3697 (1993)

Energy gap and its origin

Energy band (Bloch's theorem): energy region of extended states

Stable for small but finite perturbation

Not joking: physicists are a bit more serious

Something

to be observed & useful !

"EDGE STATES"

"Dangling bonds" exist ! when non trivial !

Bulk-edge correspondence

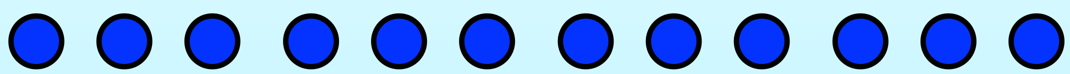
Y. H., Phys. Rev. Lett. 71, 3697 (1993)

Energy band & gap : physicist & chemist ?

Sorry if I'm wrong

physicist

itinerant electrons

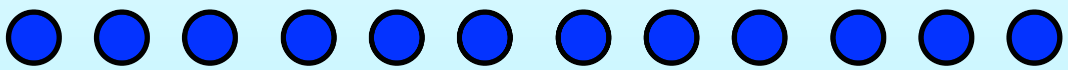


Energy band & gap : physicist & chemist ?

Sorry if I'm wrong

physicist

itinerant electrons



hopping

make energy band

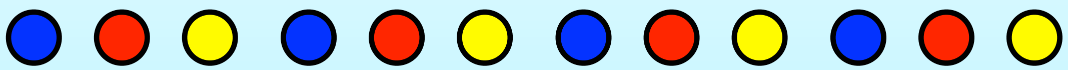
metal

Energy band & gap : physicist & chemist ?

Sorry if I'm wrong

physicist

itinerant electrons

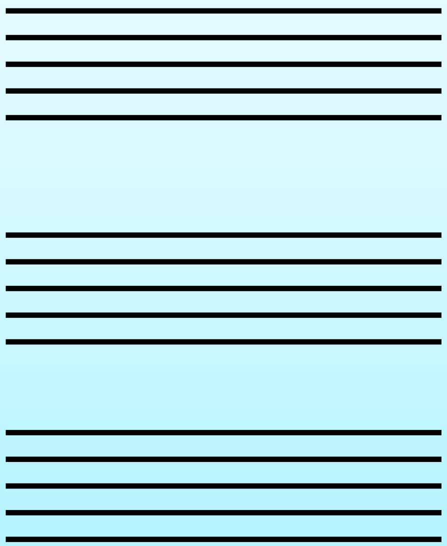


hopping

Peierls instability

Opening gap

stabilize

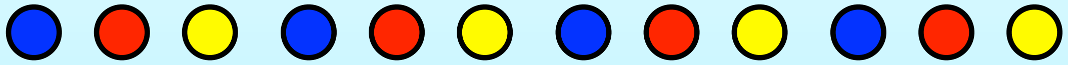


Energy band & gap : physicist & chemist ?

Sorry if I'm wrong

physicist

itinerant electrons

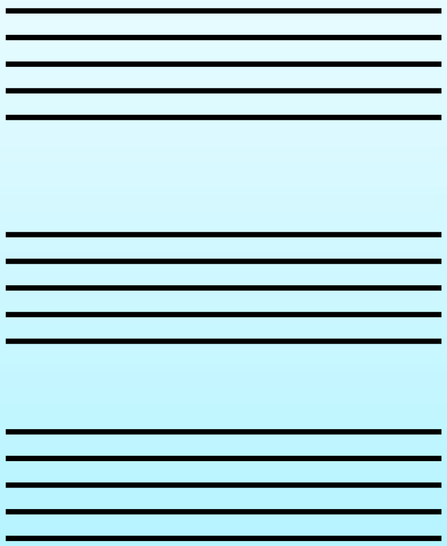


hopping

Peierls instability

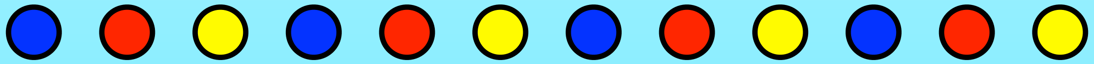
Opening gap

stabilize



chemist

form molecules first

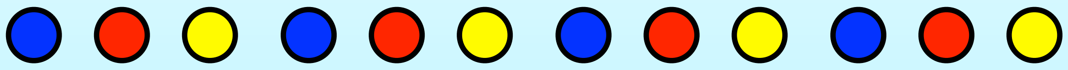


Energy band & gap : physicist & chemist ?

Sorry if I'm wrong

physicist

itinerant electrons

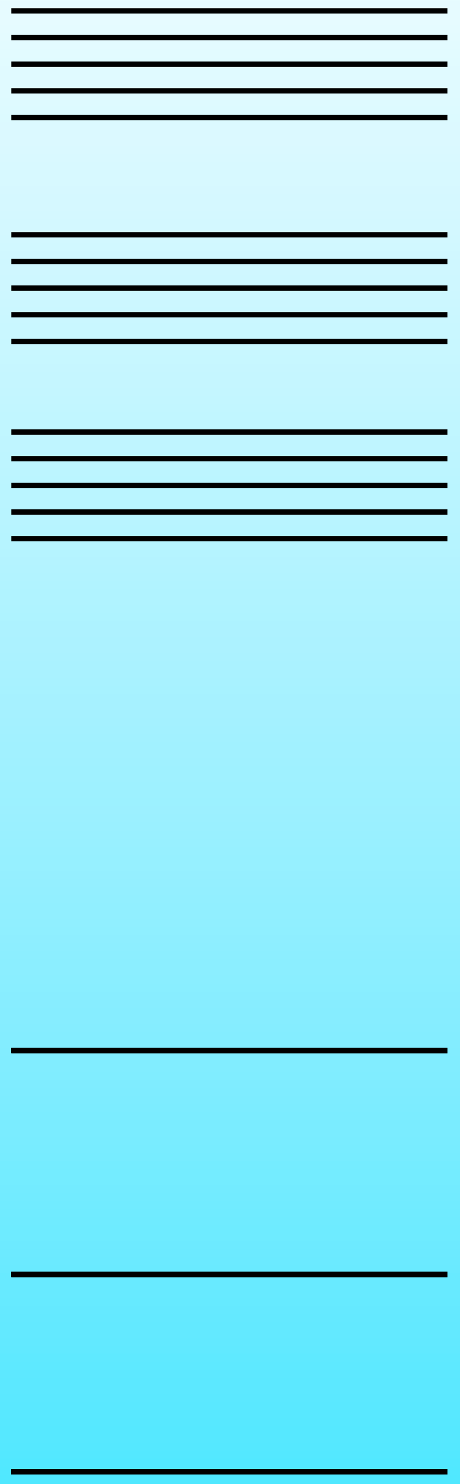


hopping

Peierls instability

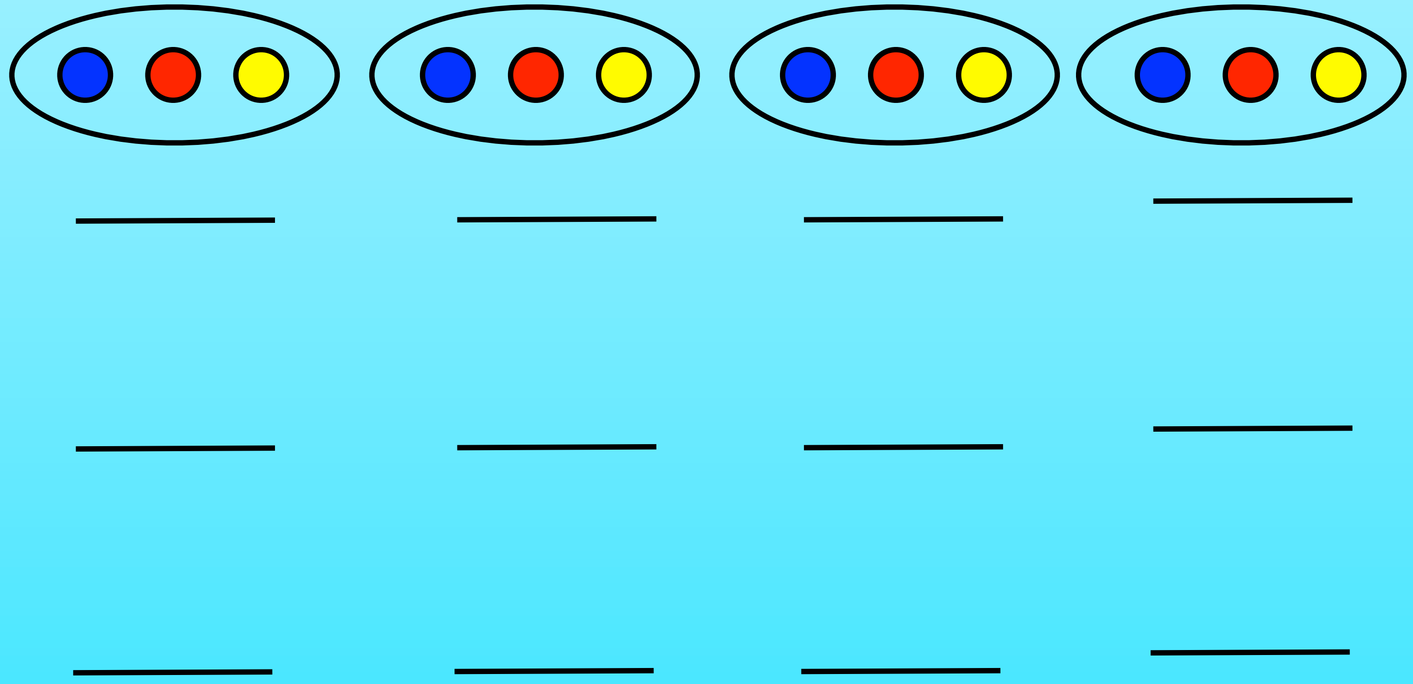
Opening gap

stabilize



chemist

form molecules first

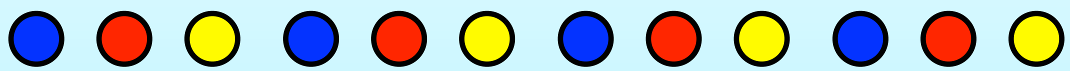


Energy band & gap : physicist & chemist ?

Sorry if I'm wrong

physicist

itinerant electrons

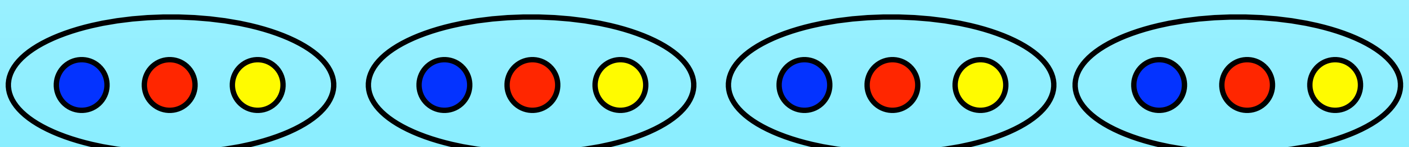


Peierls instability

stabilize

chemist

form molecules first



non orthogonality

short range entanglement

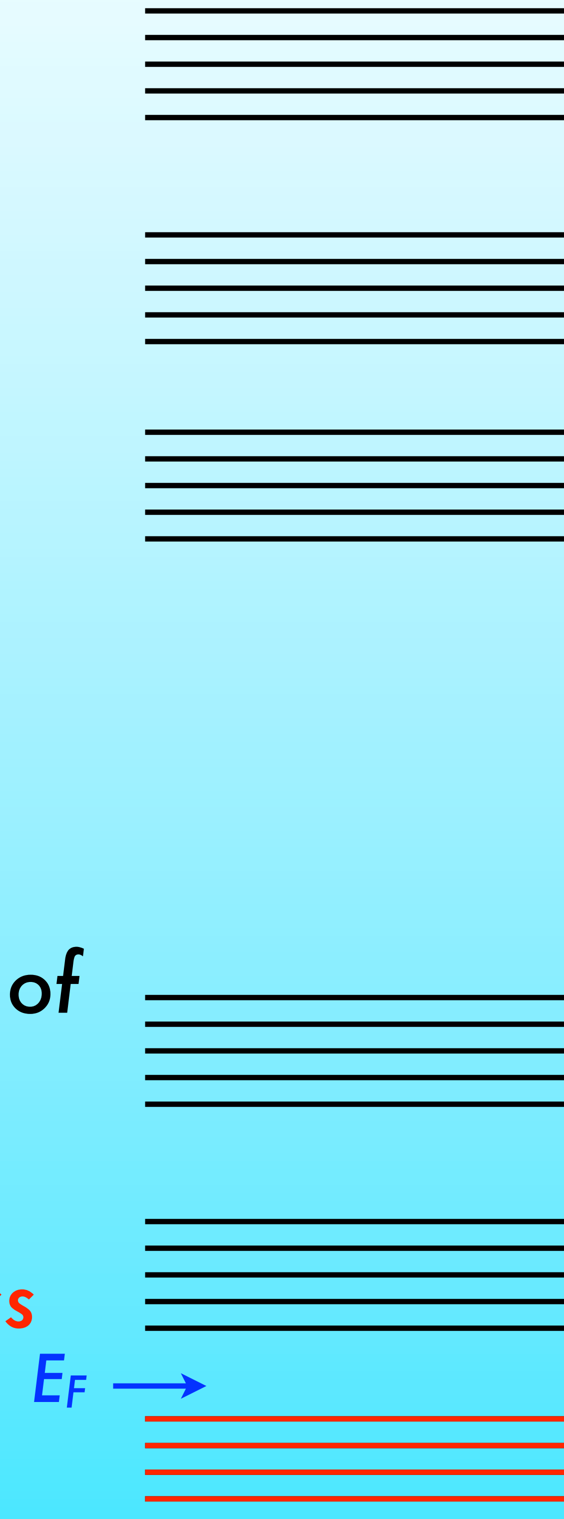
Dimer & Multimer

QUATUM Effects !

make bands of molecules

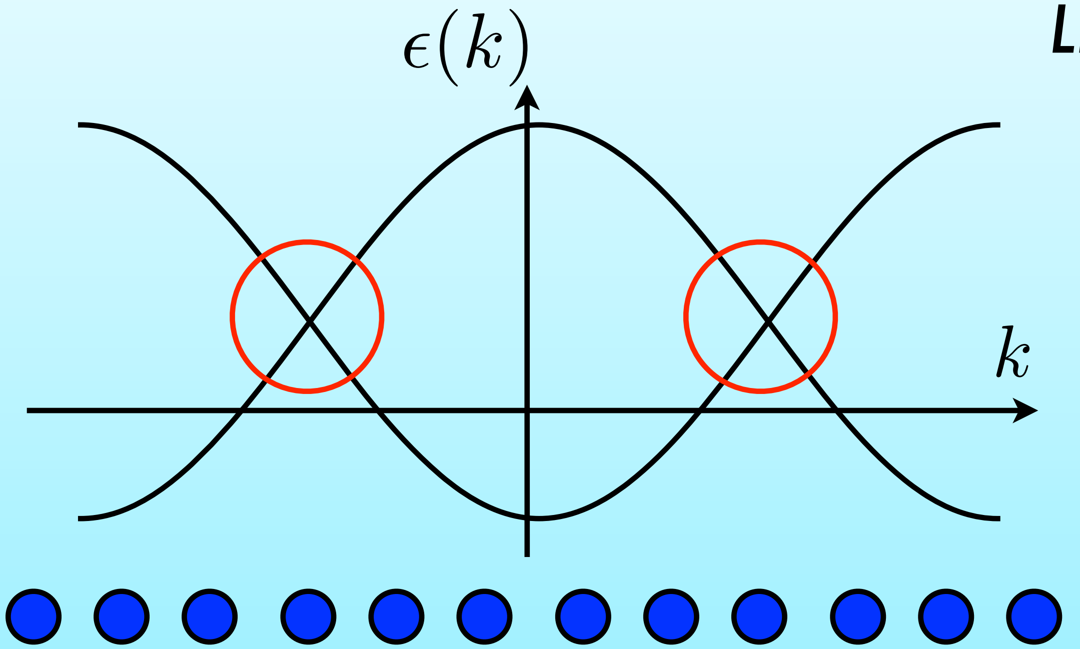
Adiabatic process

Insulator



Energy gap and Dirac fermions

Extended Brillouin zone



Linear dispersion

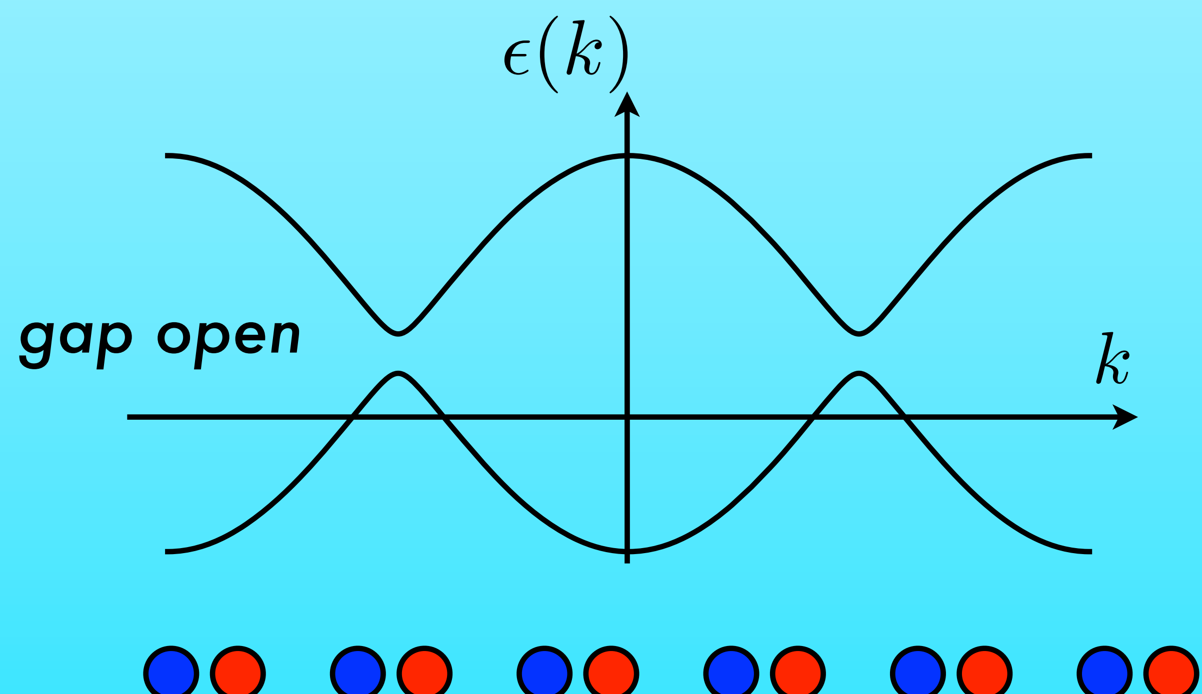
$$\epsilon(k) = \pm v_F |k|$$

1D graphene: polyacetylene

zero-gap semiconductor

Massless Dirac fermions

Fermion doubling × 2



dimerized

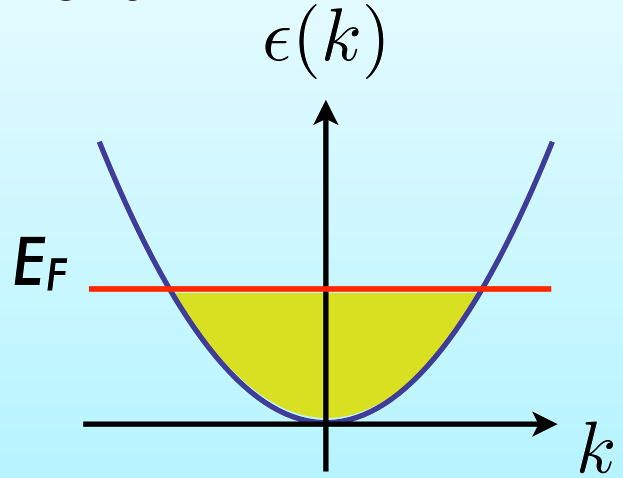
Band gap!

Massive Dirac fermions

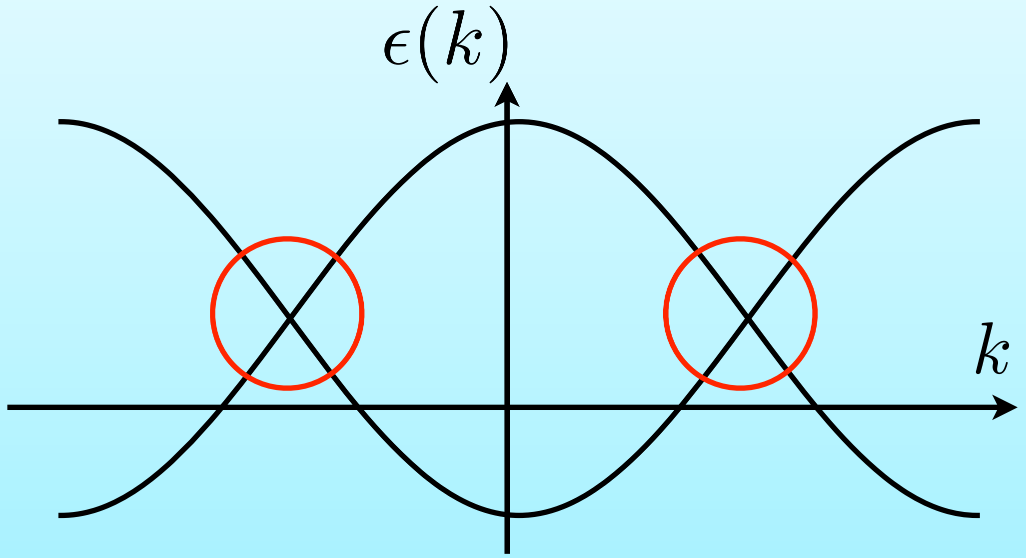
$$\epsilon(k) = \pm v_F \sqrt{k^2 + m^2}$$

Zero gap semiconductor: half electrons

Electrons



Zero gap semiconductors



$$H_{ele} \propto k^2$$

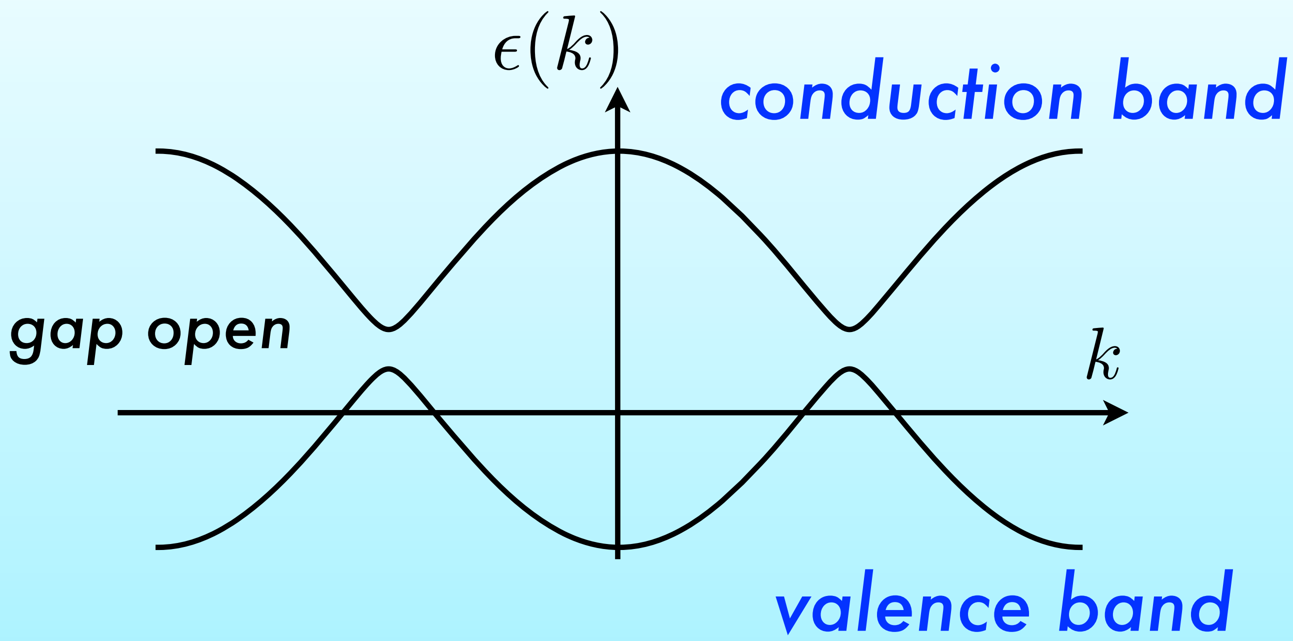
$$H_{zero} \propto |k|$$

$$\sqrt{H_{ele}} = H_{zero}$$: half electrons

$$H_{ele} = \sqrt{H_{ele}} \oplus \sqrt{H_{ele}}$$

What's band inversion ? (2D topological insulator)

2D



Massive Dirac fermions

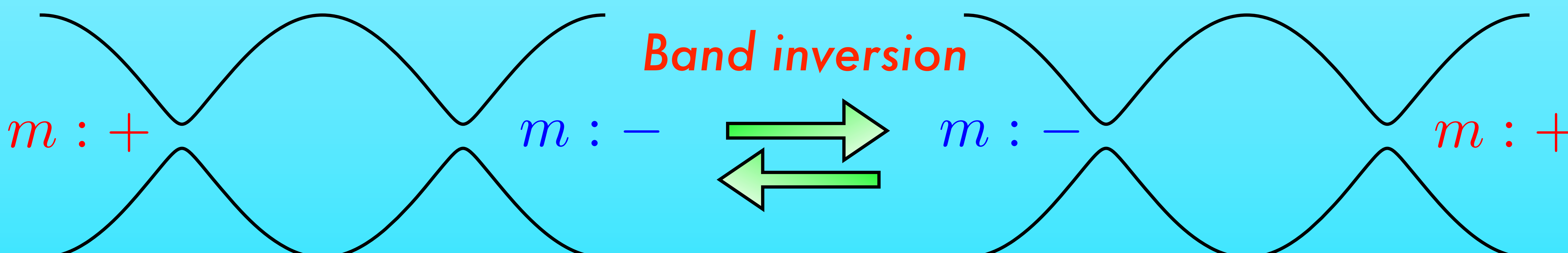
$$\epsilon(k) = \pm\sqrt{k^2 + m^2}$$

eigen values :

2 band: 2×2 matrix

$$\begin{pmatrix} m & k_x - ik_y \\ k_x + ik_y & -m \end{pmatrix}$$

m can be negative !

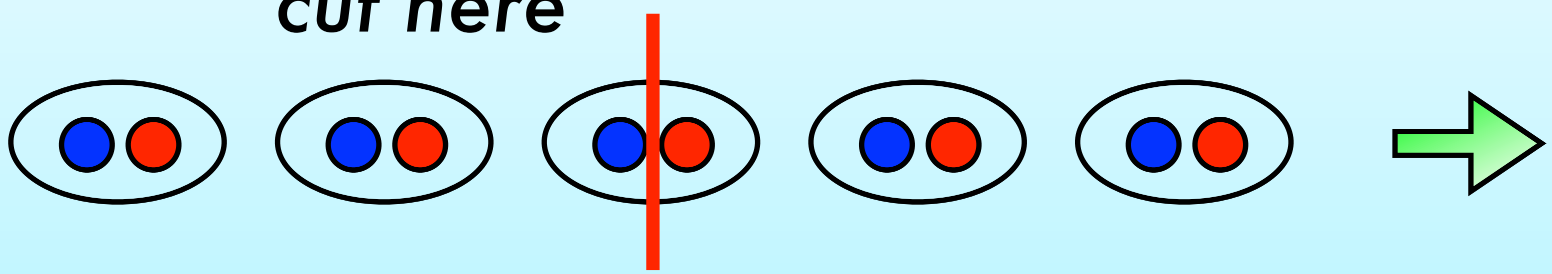


e.g. by changing width of the superlattice (HgTe-CdTe)

Appearance of edge states

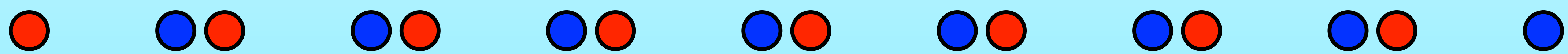
cut here

dangling bond appear



very long chain with boundaries

in-gap states are induced



without boundaries

conduction band

band gap

valence band

with boundaries

conduction band

in-gap states

valence band

dimerization pattern ⟷ how the edge states appear

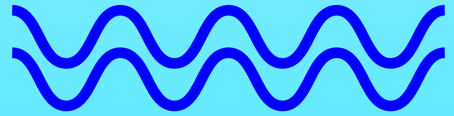
Bulk-edge correspondence

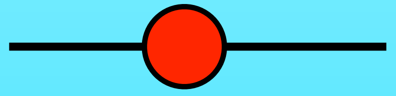
without boundaries	*with* boundaries
conduction band	*conduction band*
band gap	*in-gap states*
valence band	*valence band*

dimerization pattern ⟺ *how the edge states appear*

Bulk (before making boundaries) determines the edge states

The edge states reflect the dimerization pattern of the bulk





Bulk state *Control each other* *Edge state*

Plan

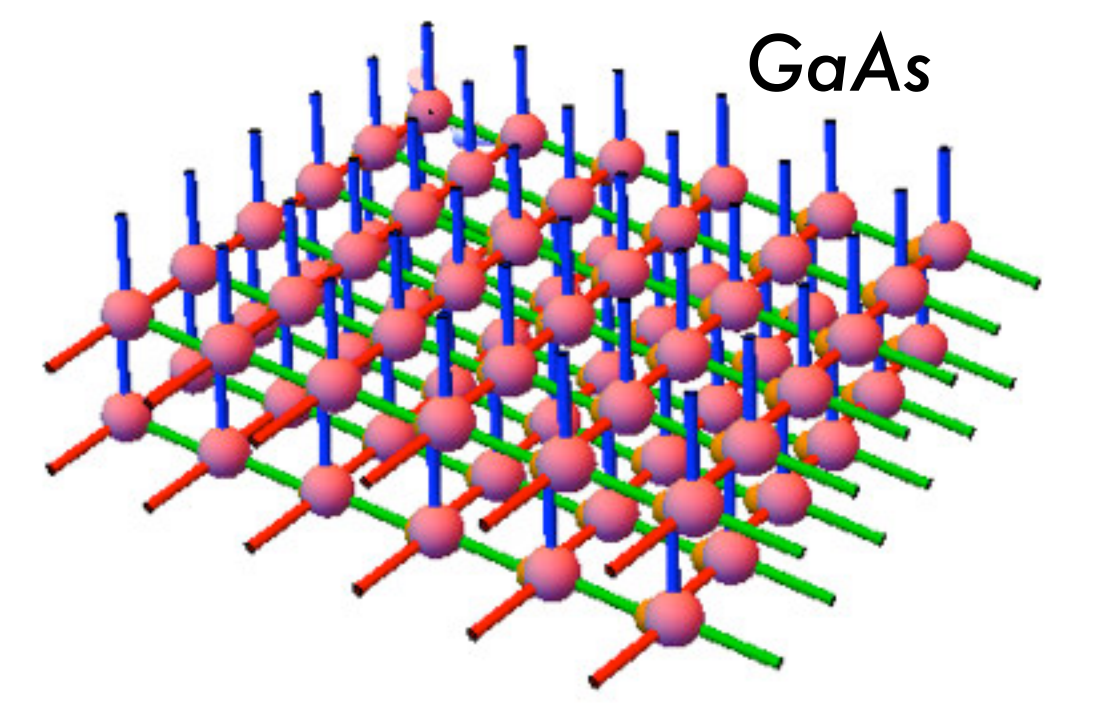
- *Metal, insulator & semiconductor*
- *Bulk-edge correspondence :graphene, silicene and more*
- *From Newton to Dirac for devices breakthrough*

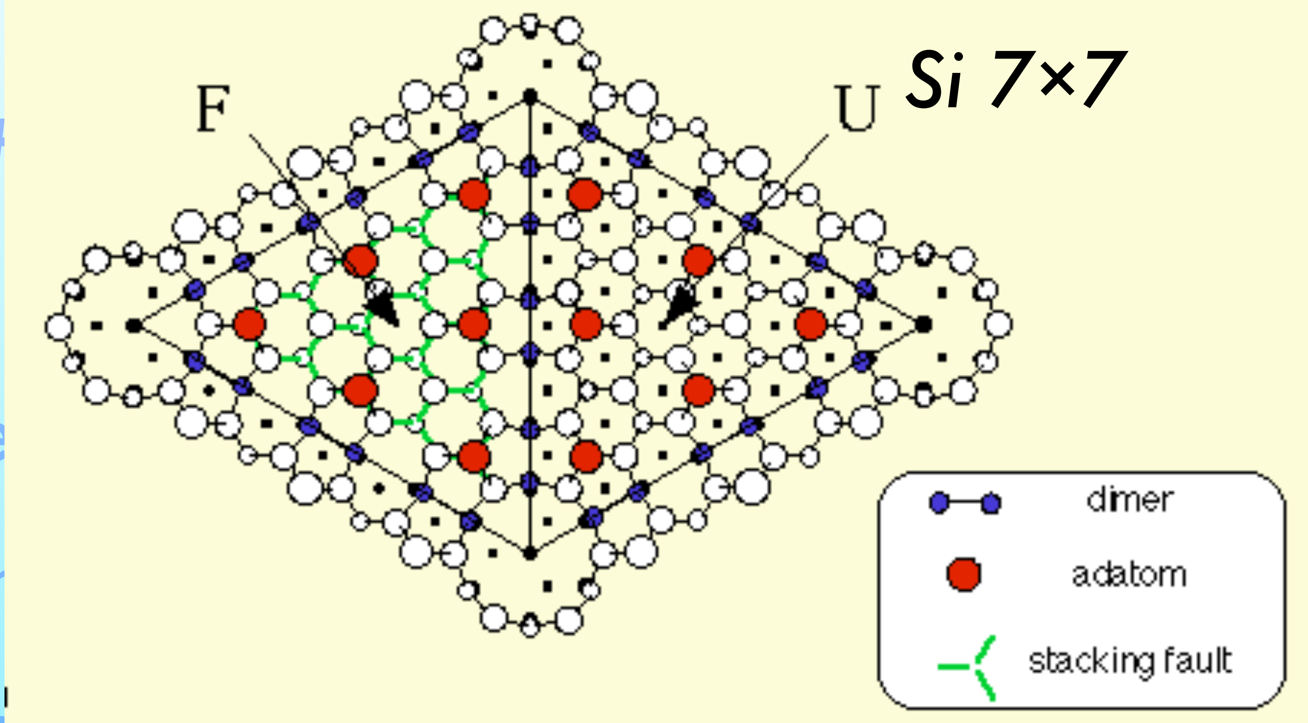
Zoo of Boundary (Edge) States in materials

From textbook examples to new discoveries

- Levinson's theorem to the Friedel's sum rule
- Surface states of Semiconductors & polarization
- Solitons in polyacetylene
- Edge states in quantum Hall effects
- Local moments in integer spin chains near the impurities
- Zero bias conductance peaks of the d-wave superconductors
- Zero energy localized states of graphene
- Zero energy localized states of silicene
- Edge states in 2D cold atoms in optical lattice
- One-way edge modes in gyromagnetic photonic crystals
- Quantum Spin Hall Edge states

☆ *Surface states of Semiconductors & polarization*





PHYSICAL REVIEW B VOLUME 47, NUMBER 3 15 JANUARY 1993-I

Theory of polarization of crystalline solids

R. D. King-Smith and David Vanderbilt

Macroscopic polarization in crystalline dielectrics: the geometric phase approach

Raffaele Resta

Reviews of Modern Physics, Vol. 66, No. 3, July 1994

+ –+ –+ –+ –+ –+ –+ –+ –+ –+ –

☆ Solitons in polyacetylene

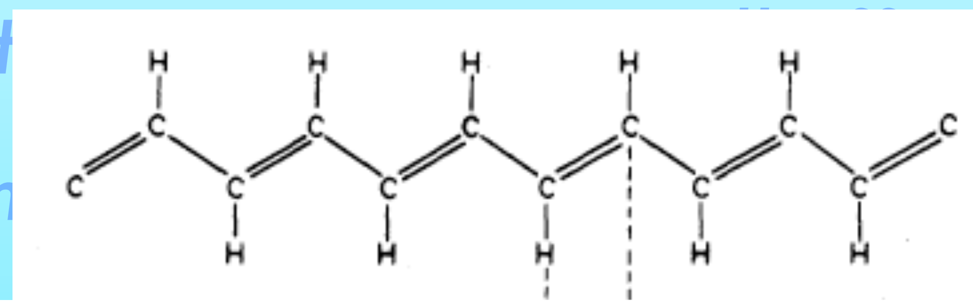
VOLUME 42, NUMBER 25 PHYSICAL REVIEW LETTERS 18 JUNE 1979

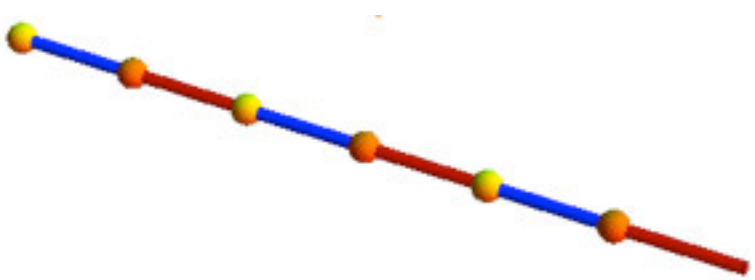
Solitons in Polyacetylene

W. P. Su, J. R. Schrieffer, and A. J. Heeger
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104
(Received 15 March 1979)

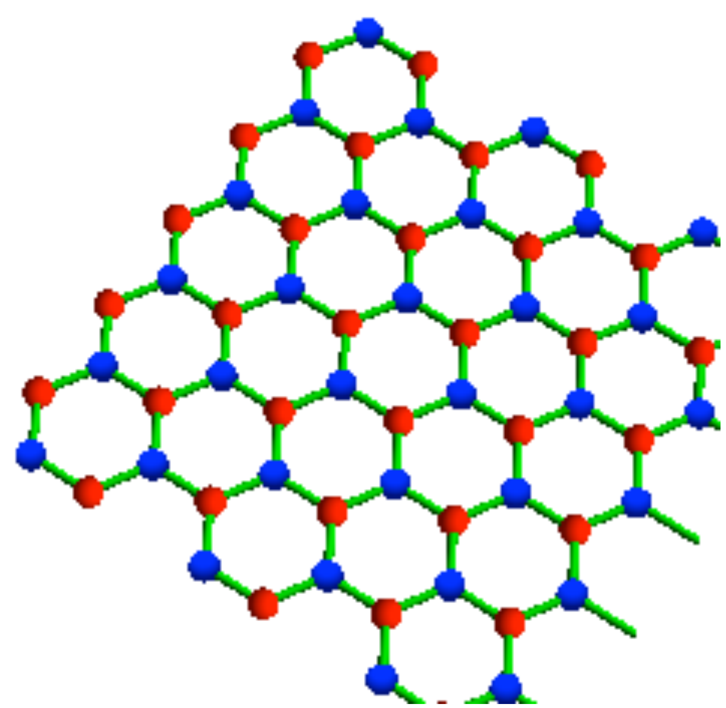
☆ Edge st … s

☆ Local m … ins near the impurities

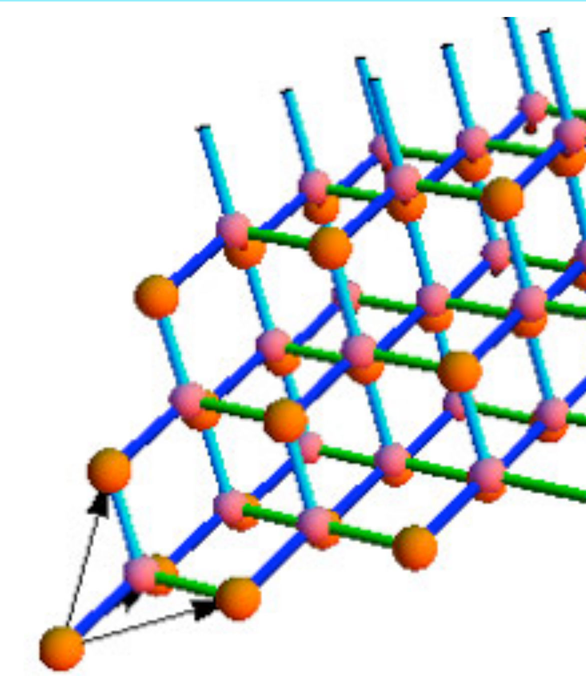




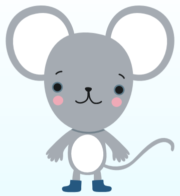
polyacetylene



graphene

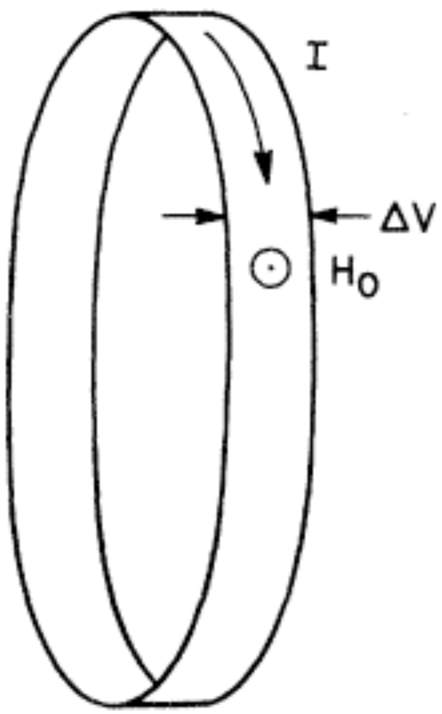


diamond



☆ Edge states in quantum Hall effects

PHYSICAL REVIEW B VOLUME 23, NUMBER 10 15 MAY 1981



Quantized Hall conductivity in two dimensions

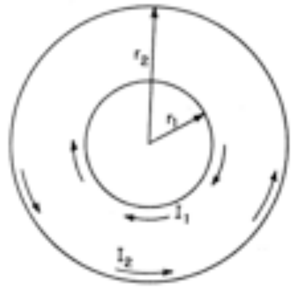
R. B. Laughlin
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 20 January 1981)

Everything started from here

PHYSICAL REVIEW B VOLUME 25, NUMBER 4 15 FEBRUARY 1982

Quantized Hall conductance, current-carrying edge states, and the existence of extended states in a two-dimensional disordered potential

B. I. Halperin

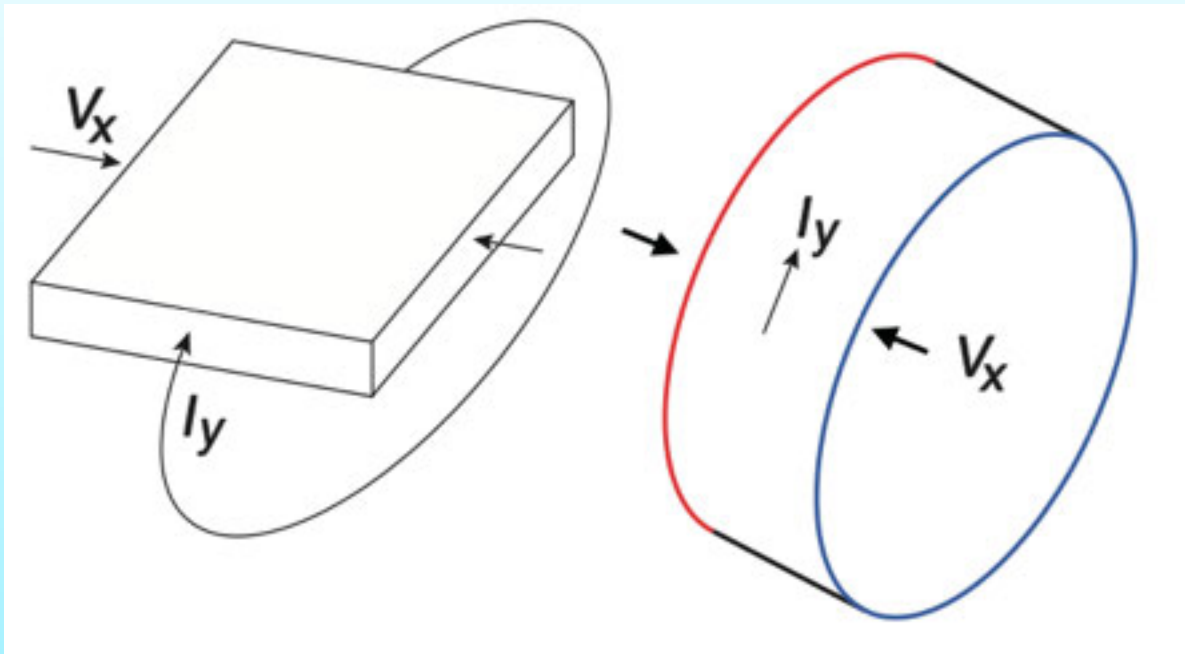


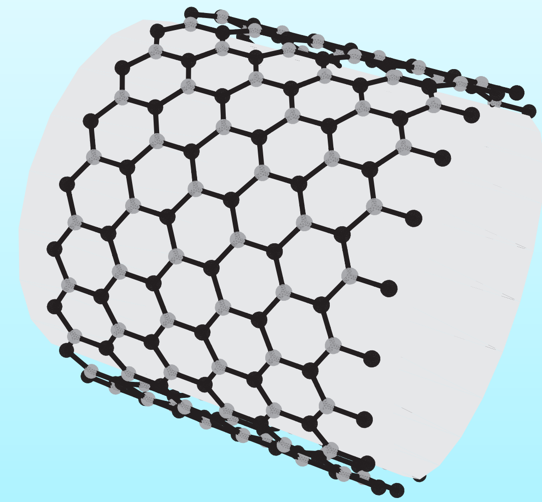
PHYSICAL REVIEW B VOLUME 48, NUMBER 16 15 OCTOBER 1993-II

Edge states in the integer quantum Hall effect and the Riemann surface of the Bloch function

Yasuhiro Hatsugai*

Hall Conductance has double Topological meanings





$$\sigma_{xy}{}^{\text{bulk}} = \sigma_{xy}{}^{\text{edge}}$$

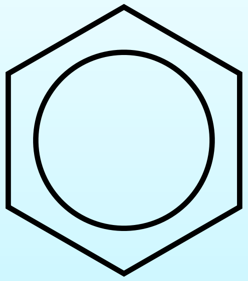
Y. Hatsugai, Phys. Rev. Lett. 71, 3697 (1993)

Y. Hatsugai, T.Fukui, H.Aoki, Phys. Rev. B. 74, 205414 (2006)

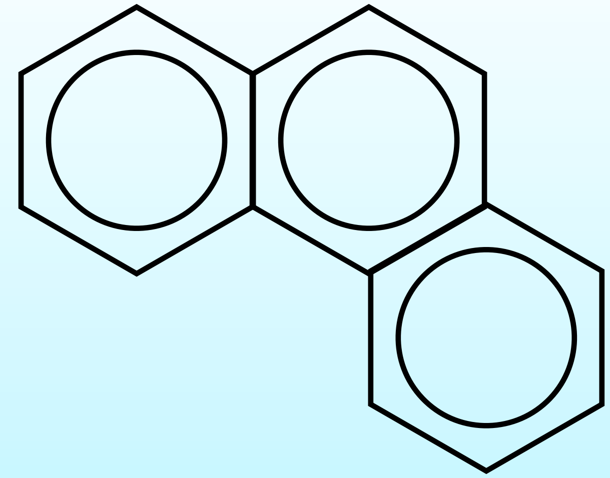
Bulk-edge correspondence

Graphene??

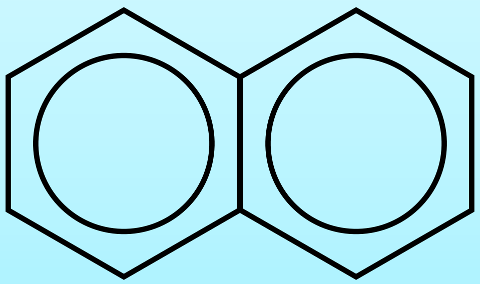
- π-electron systems



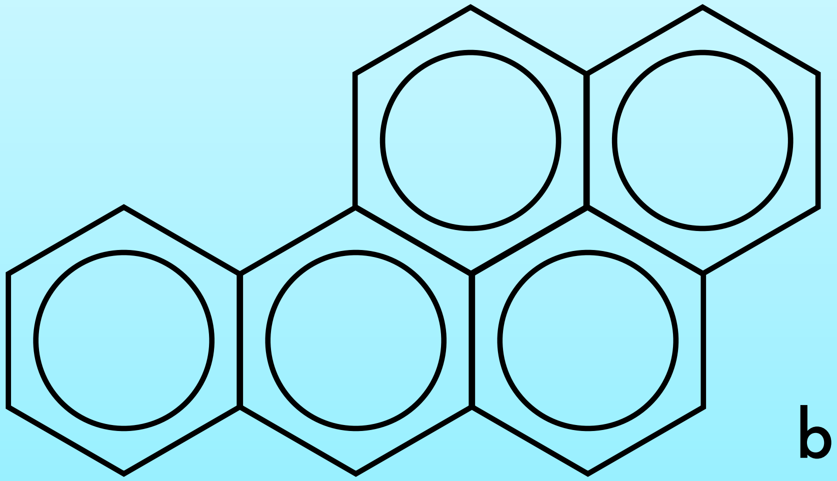
benzene



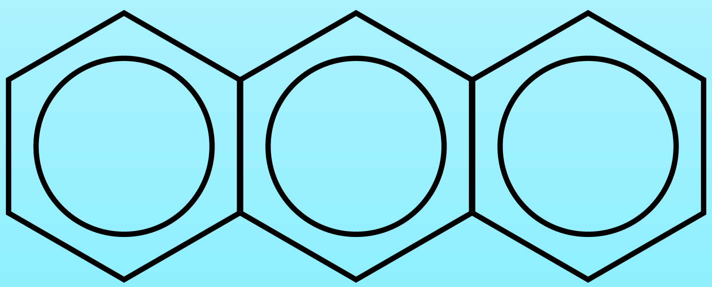
phenanthrene



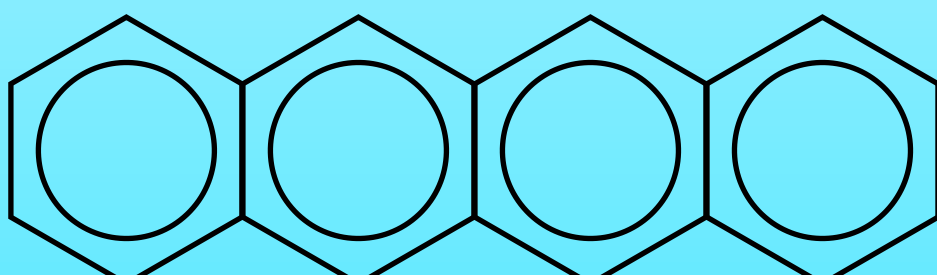
naphthalene



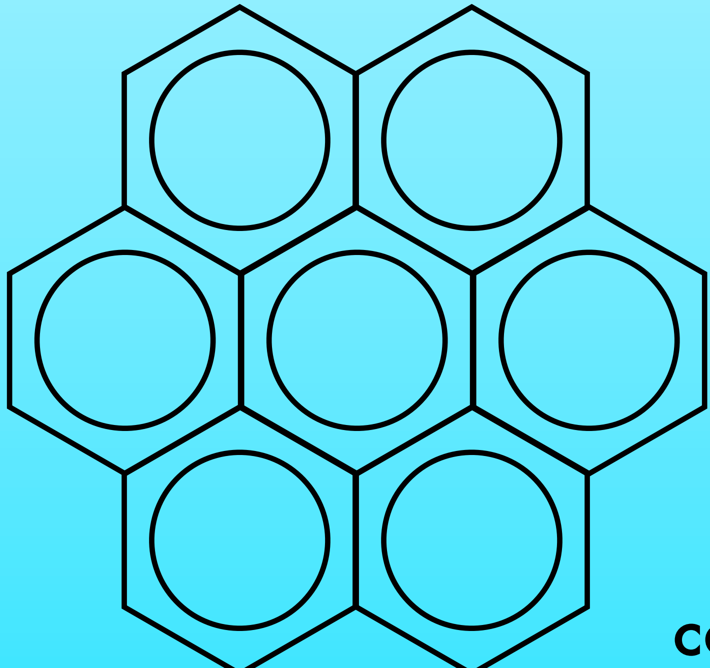
benzopyrene



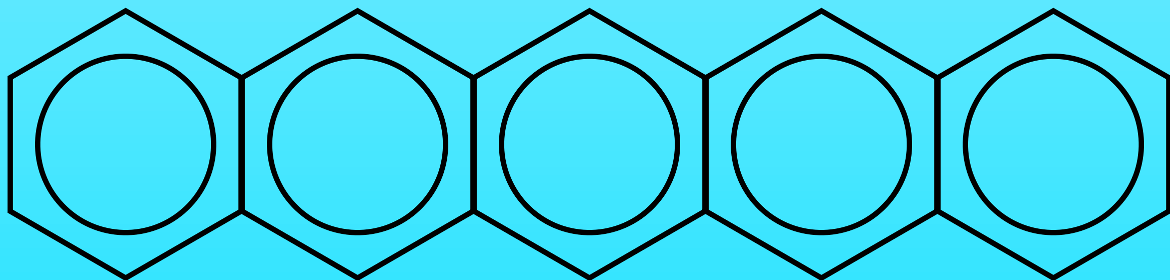
anthracene



tetracene

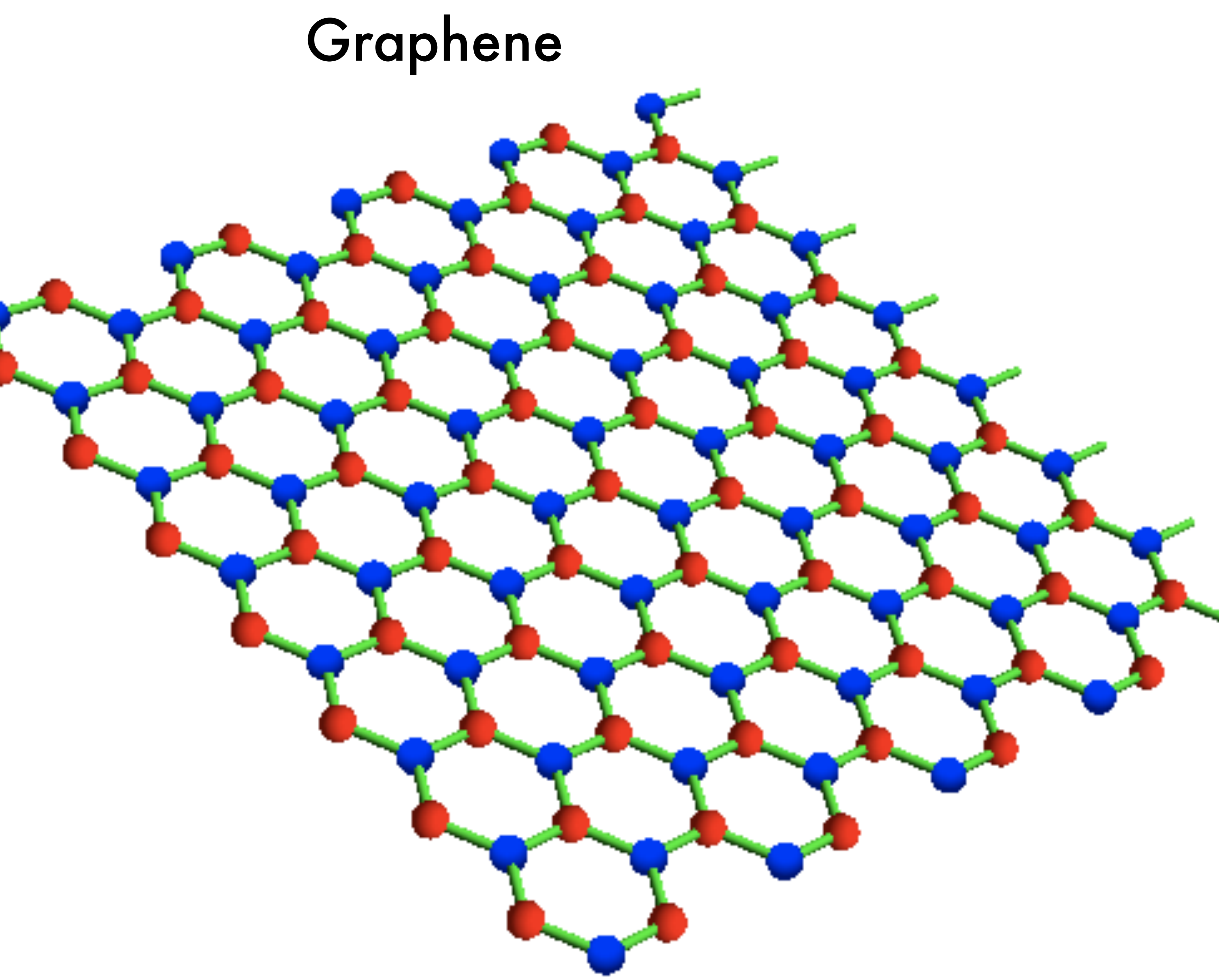


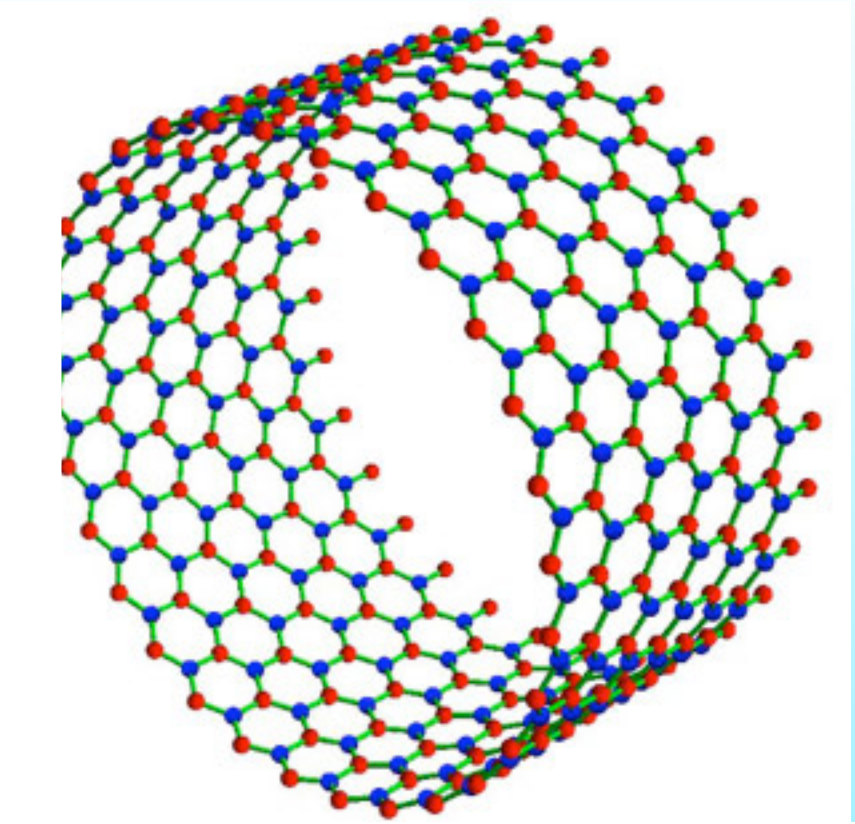
coronene

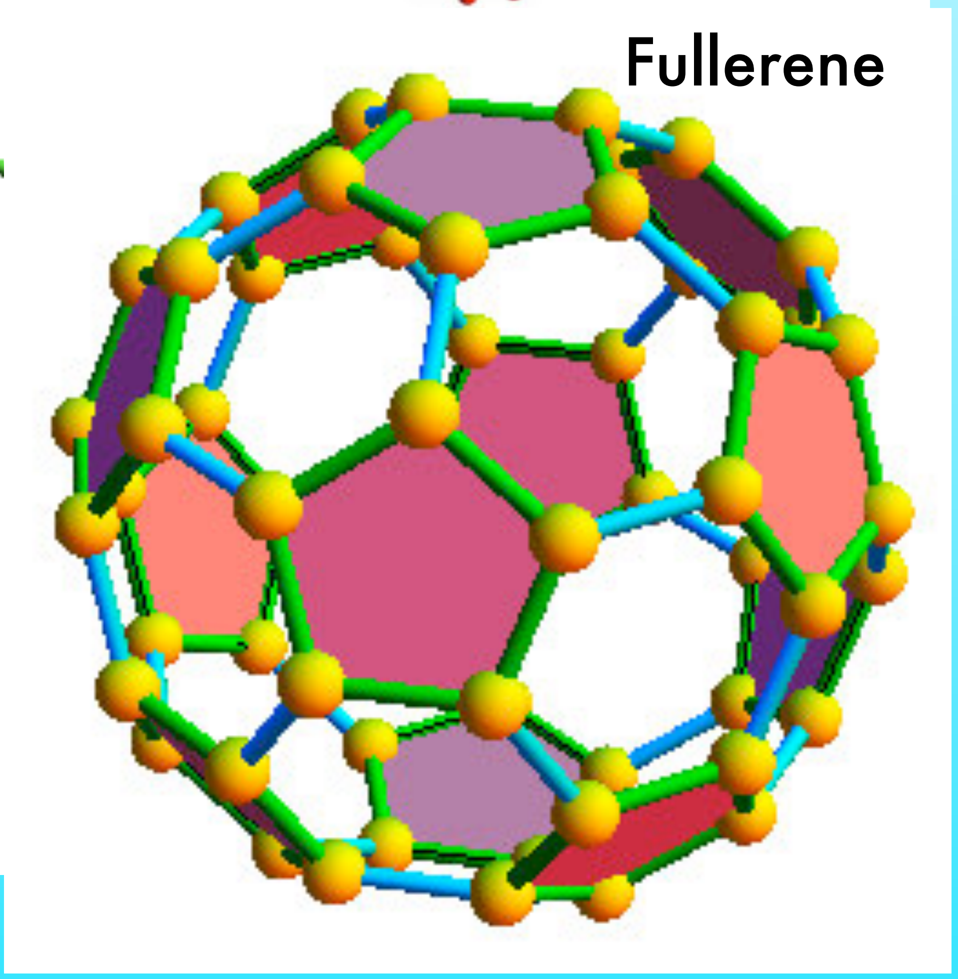


pentacene

Graphene??

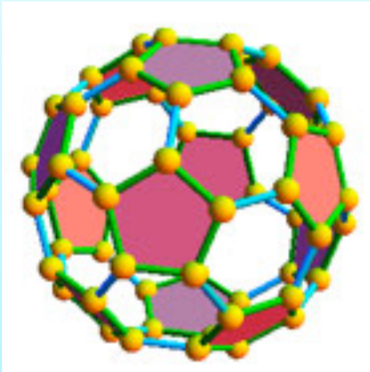






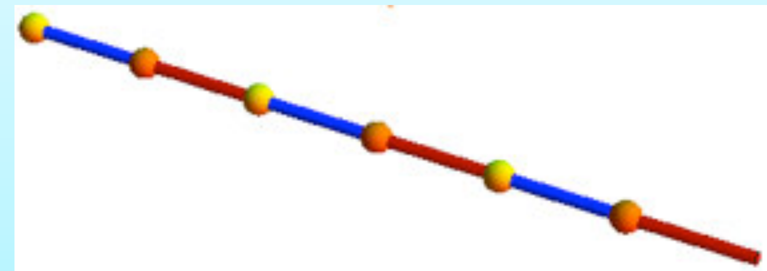
Carbons in Dimensions 0,1,2,3,...

fullerene D=0



The Nobel Prize in Chemistry 1996
Robert F. Curl Jr., Sir Harold Kroto, Richard E. Smalley

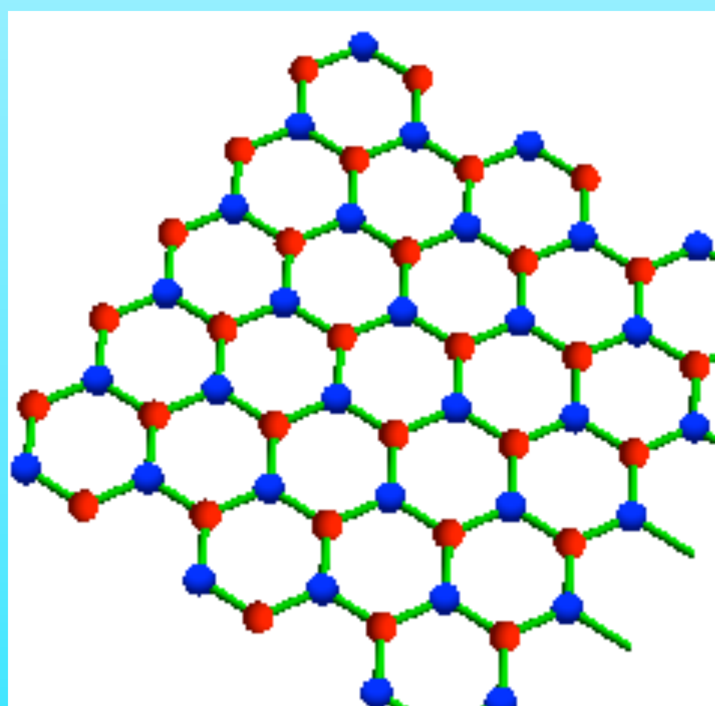
polyacetylene D=1



The Nobel Prize in Chemistry 2000
Alan Heeger, Alan G. MacDiarmid, Hideki Shirakawa

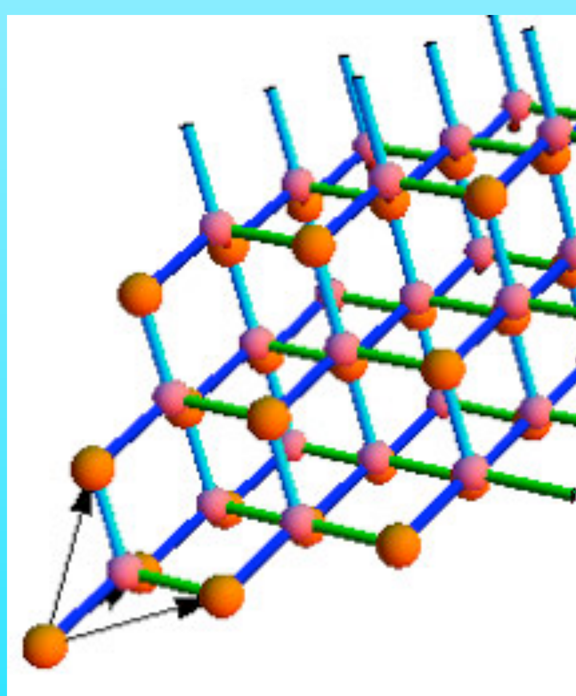
graphene

D=2 : tricky & lucky dim. for physicists



The Nobel Prize in Physics 2010
Andre Geim, Konstantin Novoselov

diamond D=3



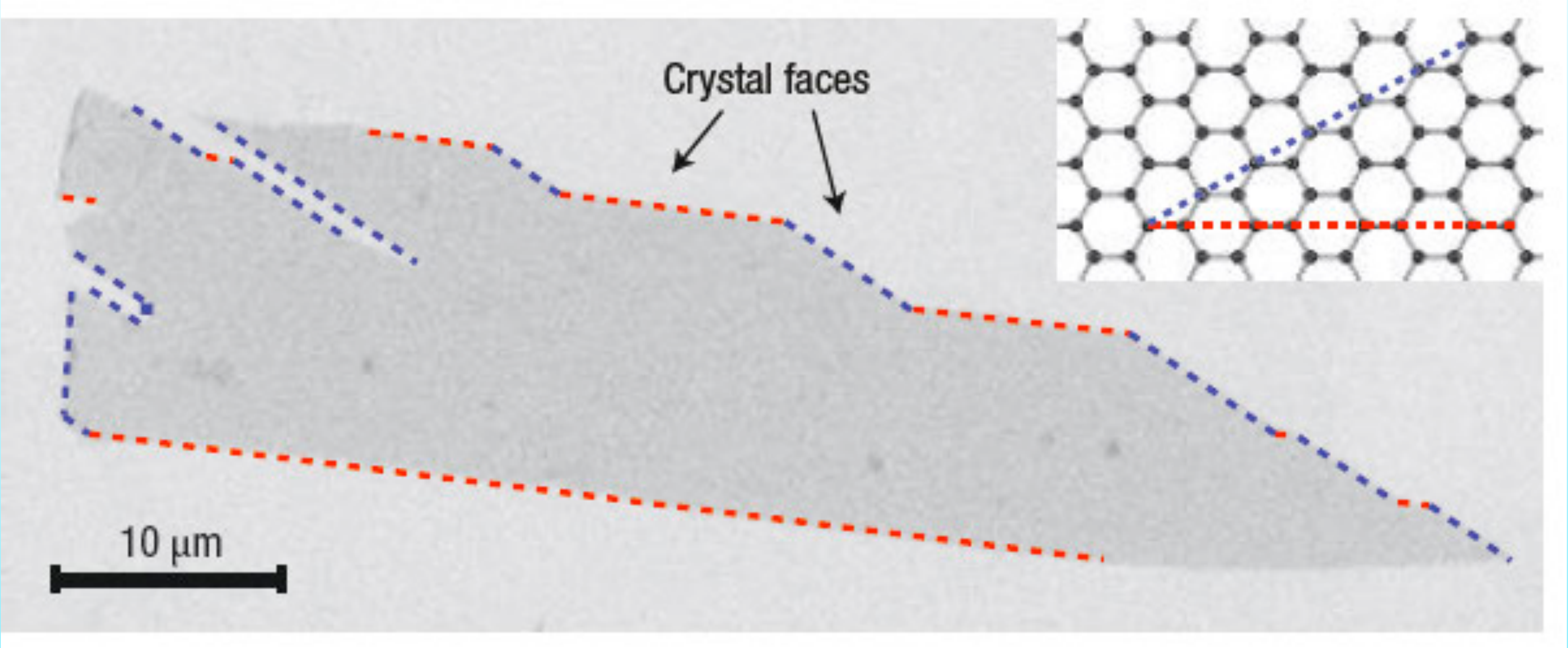
4 D graphene for lattice gauge theory

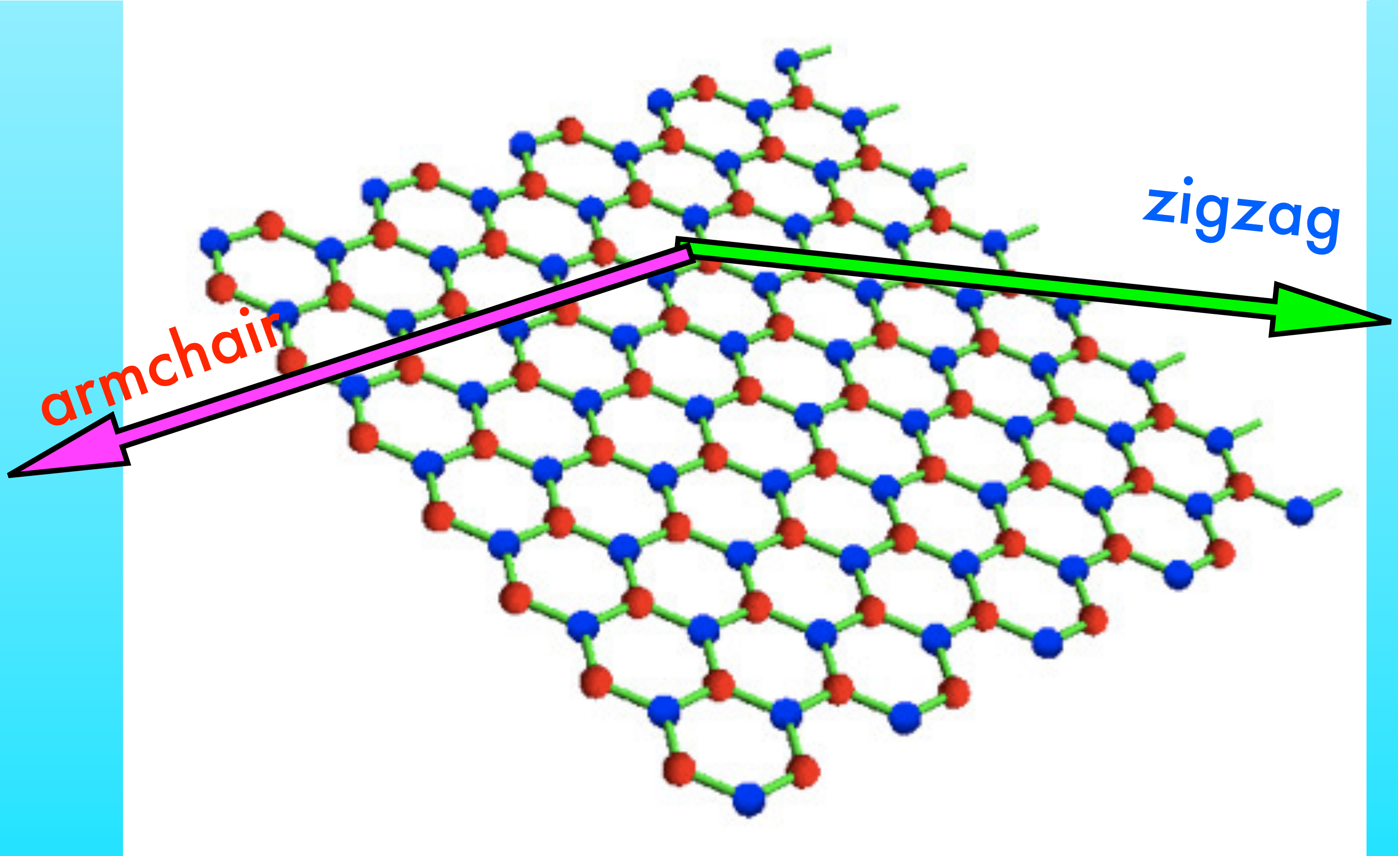
M.Creutz

JHEP04(2008)017

Graphene crystal

A.Geim & K. Novoselov, Nat. Mat. 6, 183 (2007)



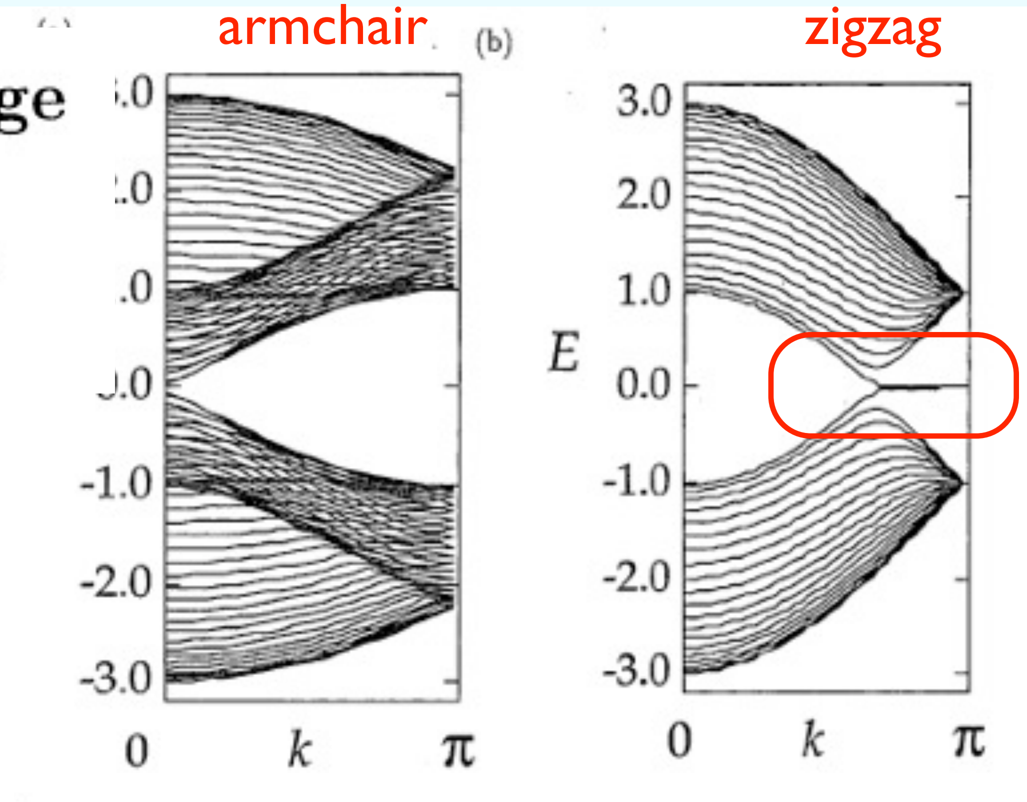


☆ Zero energy localized states of graphene

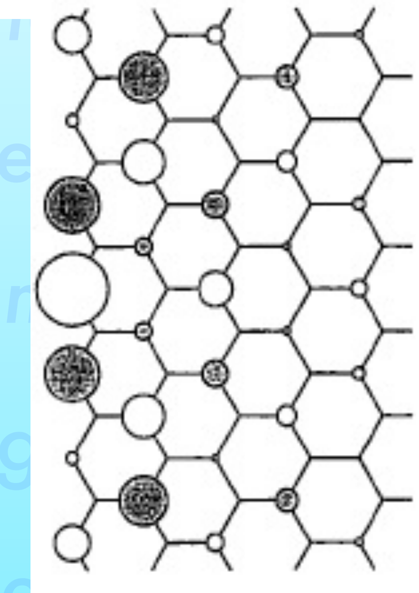
Peculiar Localized State at Zigzag Graphite Edge

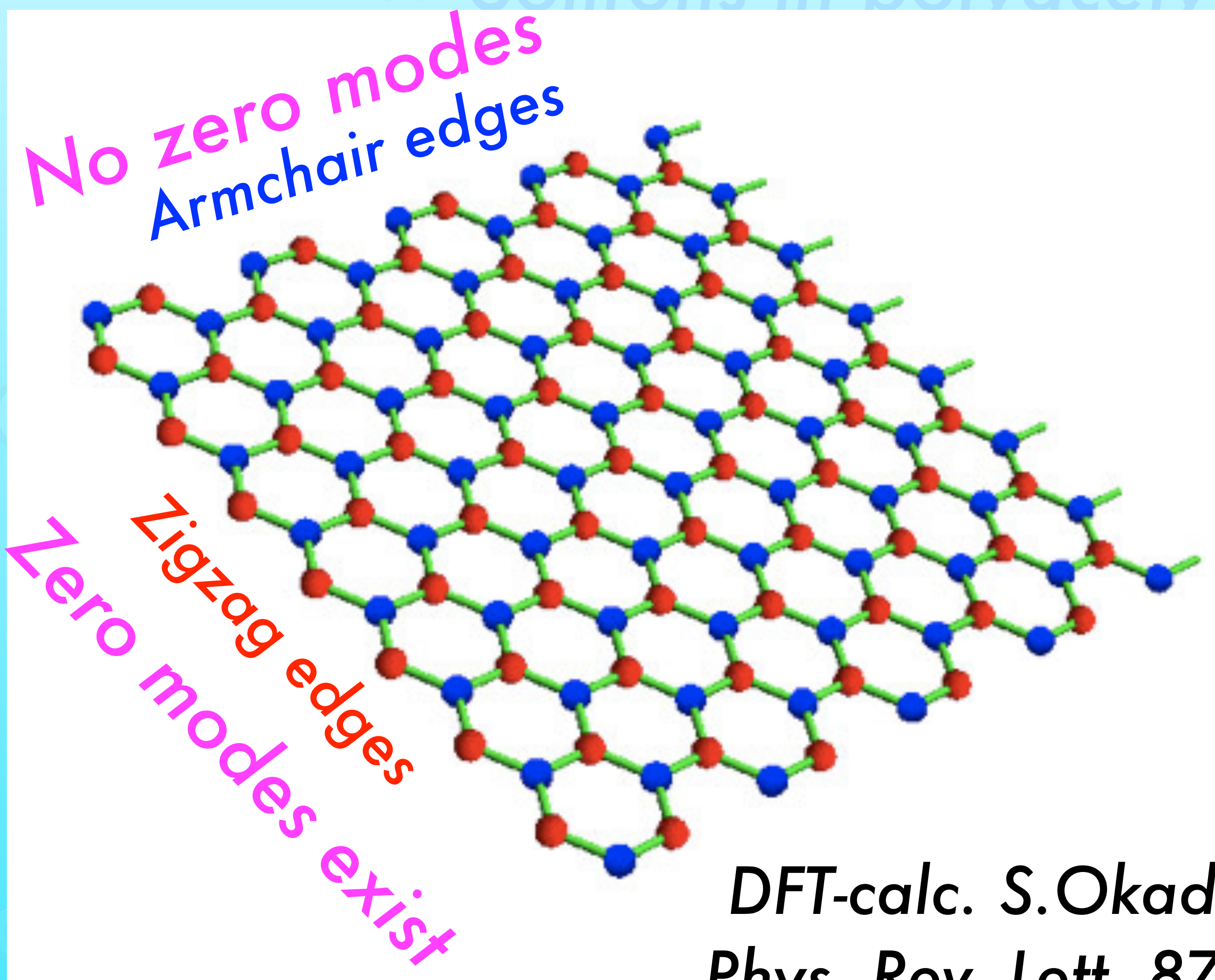
Mitsutaka FUJITA, Katsunori WAKABAYASHI, Kyoko NAKADA and Koichi KUSAKABE[1]

Journal of the Physical Society of Japan
Vol. 65, No. 7, July, 1996, pp. 1920-1923



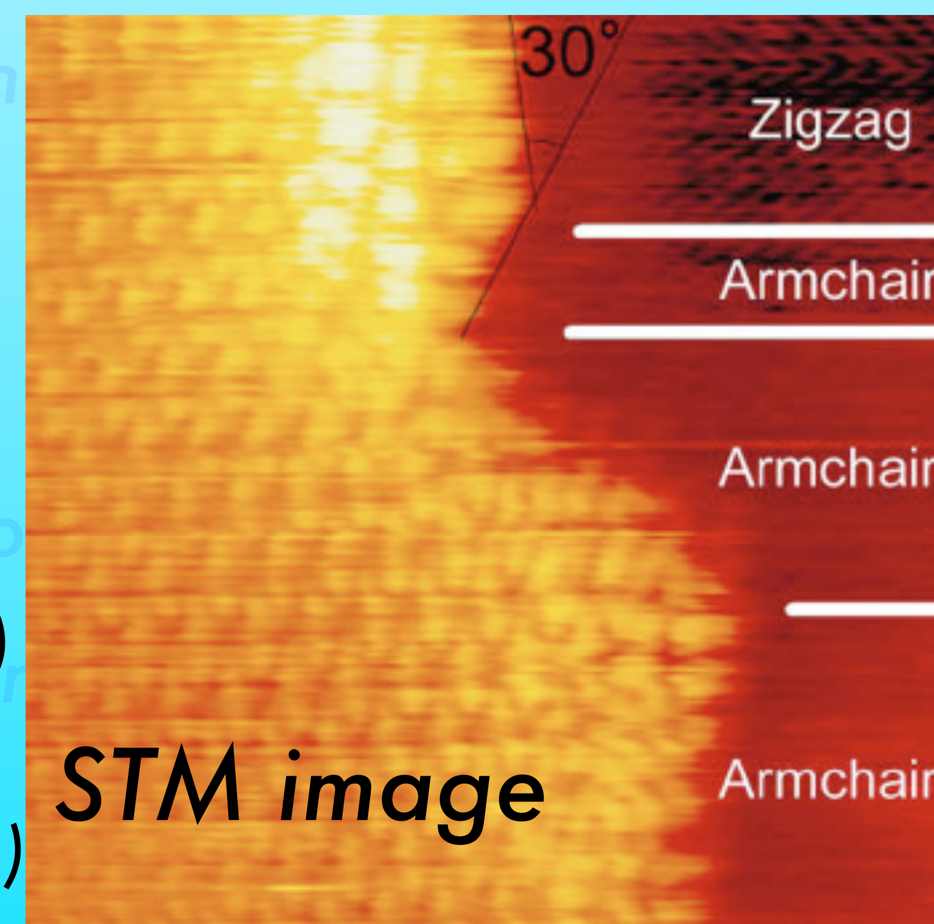
Band structure of (a) armchair and (b) zigzag ri



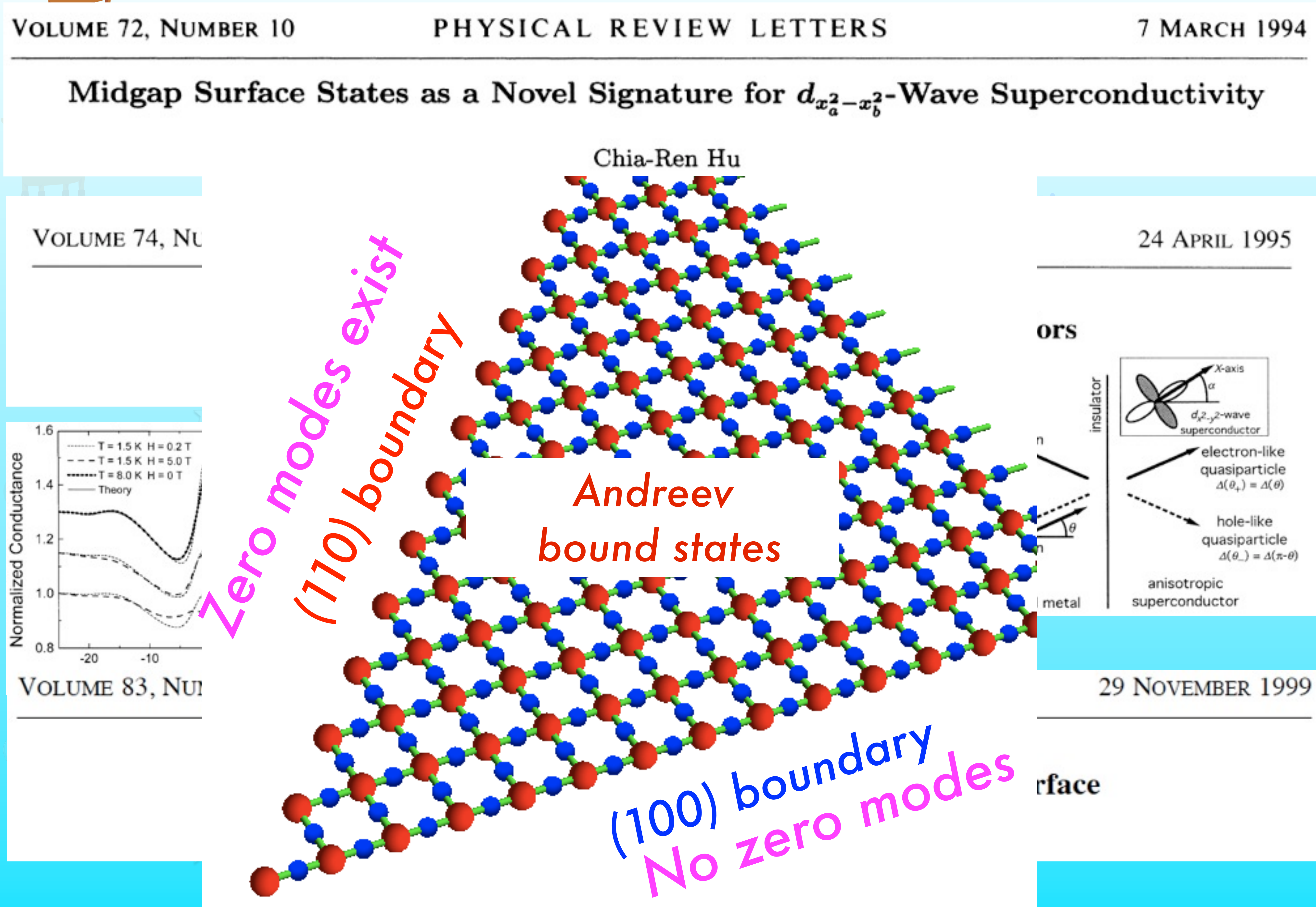


DFT-calc. S.Okada, A.Oshiyama, Phys. Rev. Lett. 87, 146803 (2001)

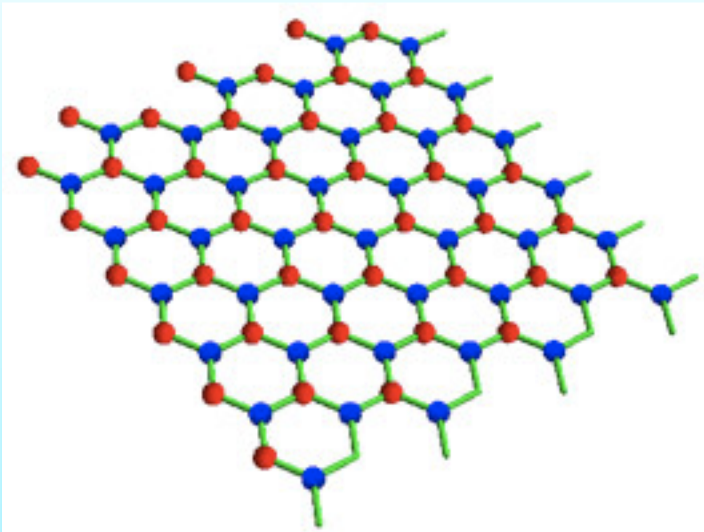
Kobayashi et al, Phys. Rev. B71, 193406 (2005)

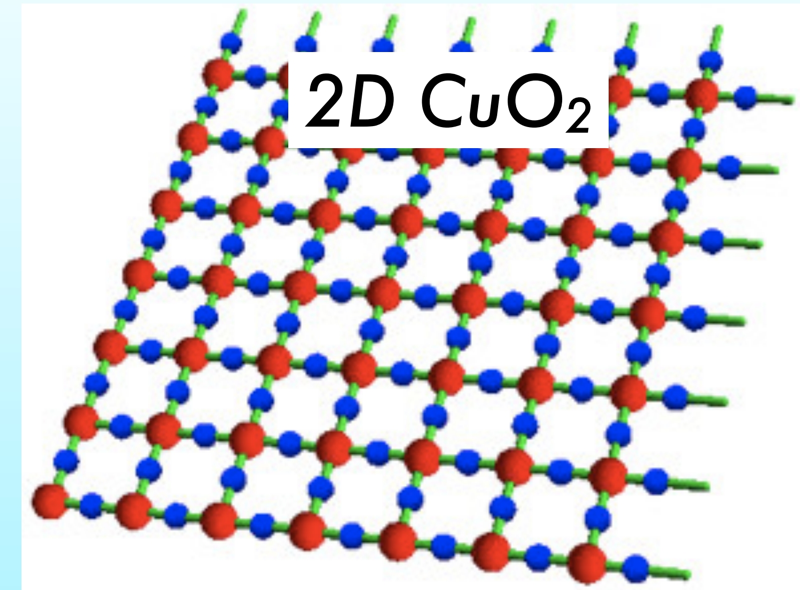


☆ Zero bias conductance peaks of the d-wave superconductors



Universality in the zero modes of Dirac Fermions

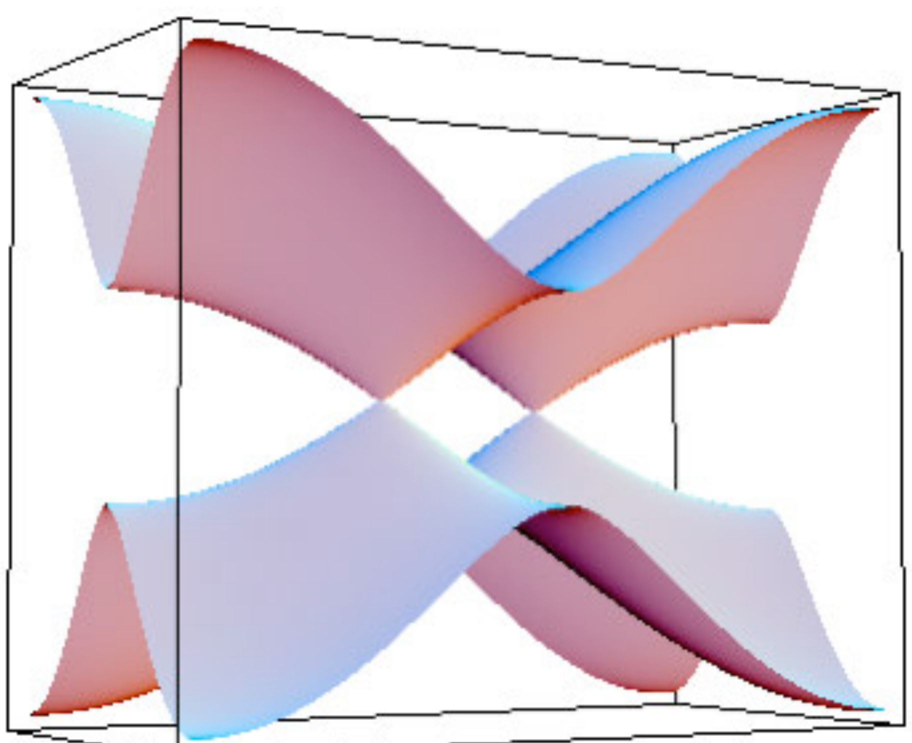




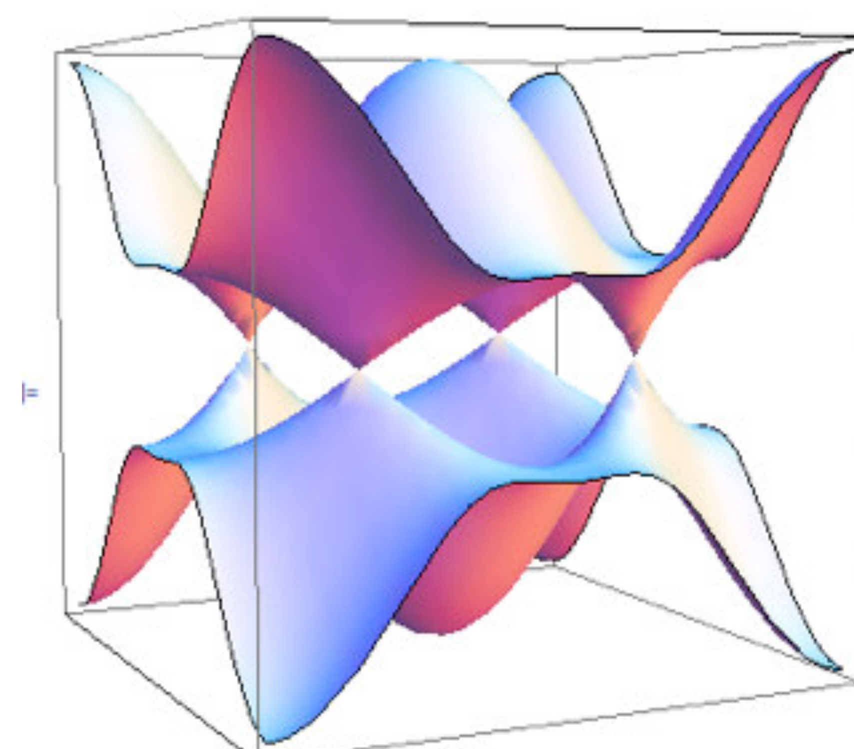
Bulk ⟺ Edge

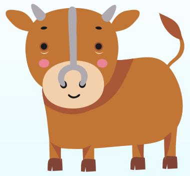
S.Ryu & Y.H., Phys. Rev. Lett. 89, 077002 (2002)
Y.H., Solid.State Comm. 149, 1061 (2009)

Graphene



d-wave superconductor



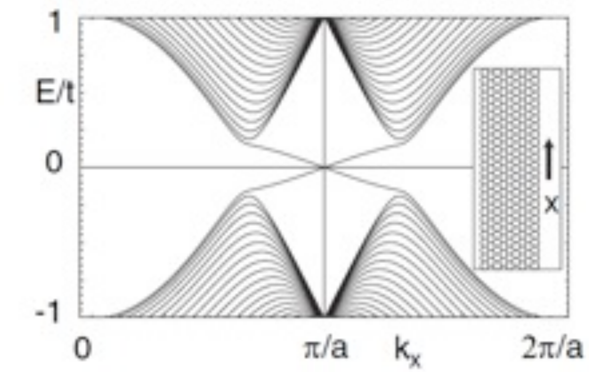


☆ Quantum Spin Hall Edge states

PRL 95, 226801 (2005) PHYSICAL REVIEW LETTERS week ending 25 NOVEMBER 2005

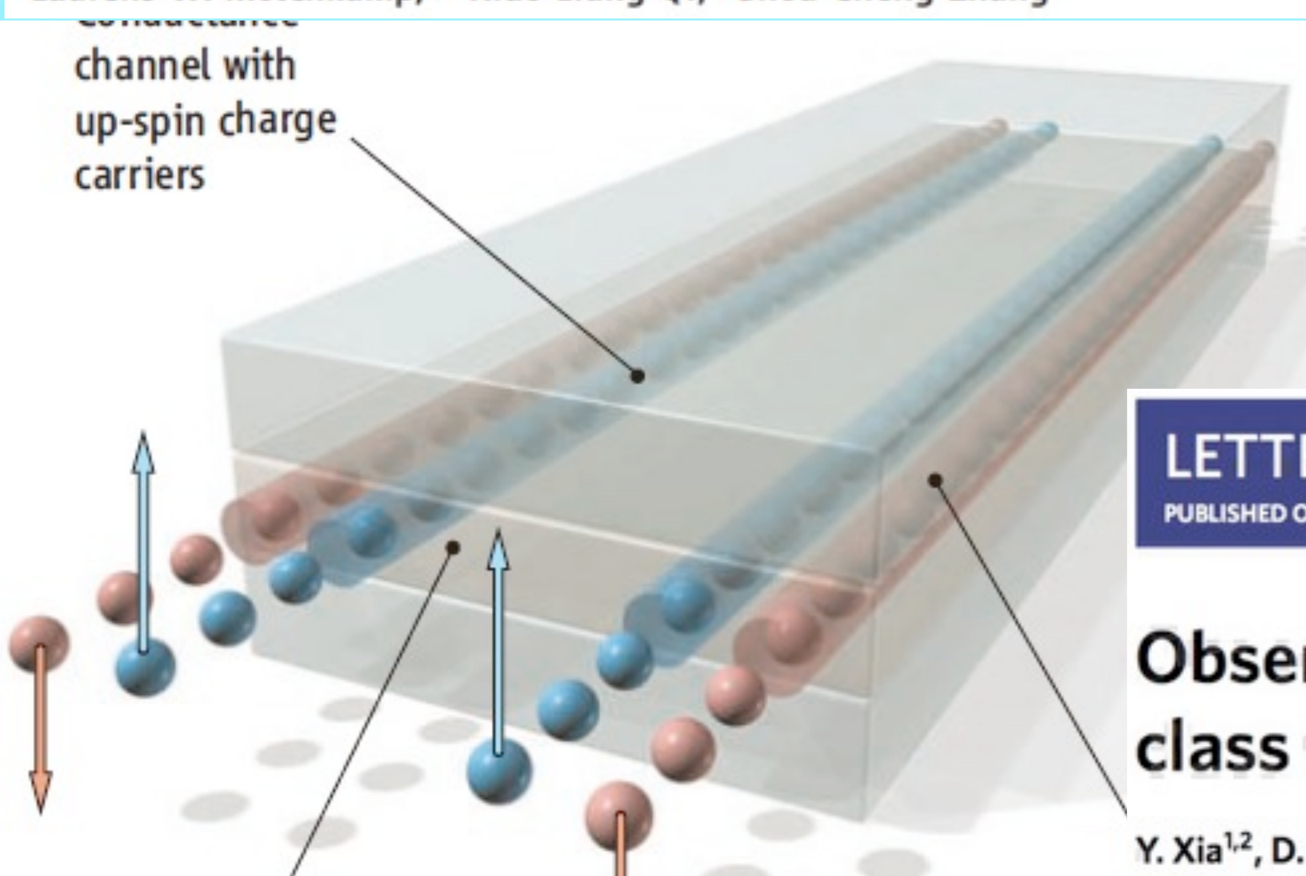
Quantum Spin Hall Effect in Graphene

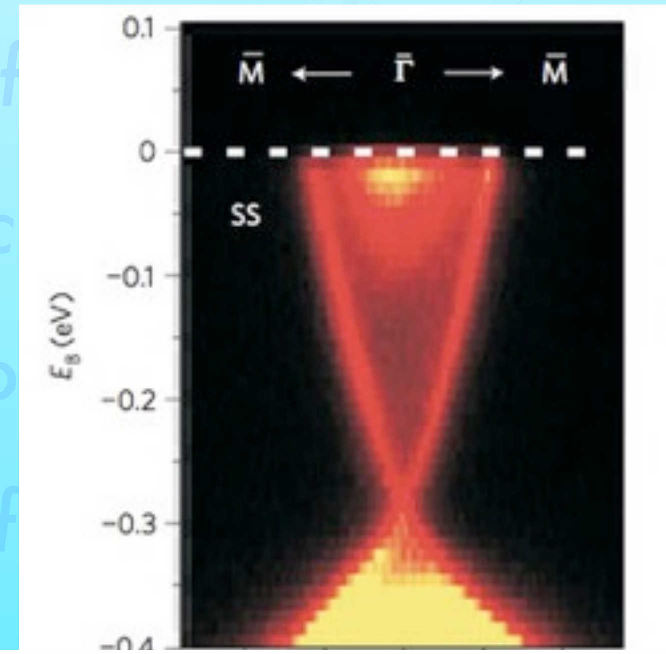
C. L. Kane and E. J. Mele

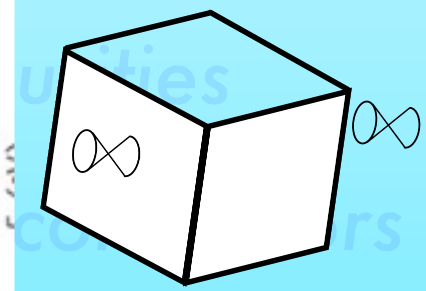


Quantum Spin Hall Insulator State in HgTe Quantum Wells

Markus König,[1] Steffen Wiedmann,[1] Christoph Brüne,[1] Andreas Roth,[1] Hartmut Buhmann,[1] Laurens W. Molenkamp,[1]* Xiao-Liang Qi,[2] Shou-Cheng Zhang[2]







LETTERS
PUBLISHED ONLINE: 10 MAY 2009 | DOI: 10.1038/NPHYS1274
nature physics

Observation of a large-gap topological-insulator class with a single Dirac cone on the surface

Y. Xia[1,2], D. Qian[1,3], D. Hsieh[1,2], L. Wray[1], A. Pal[1], H. Lin[4], A. Bansil[4], D. Grauer[5], Y. S. Hor[5], R. J. Cava[5] and M. Z. Hasan[1,2,6]★

☆ Edge states in 2D cold atoms in optical lattice

PRL **108,** 255303 (2012) PHYSICAL REVIEW LETTERS week ending 22 JUNE 2012

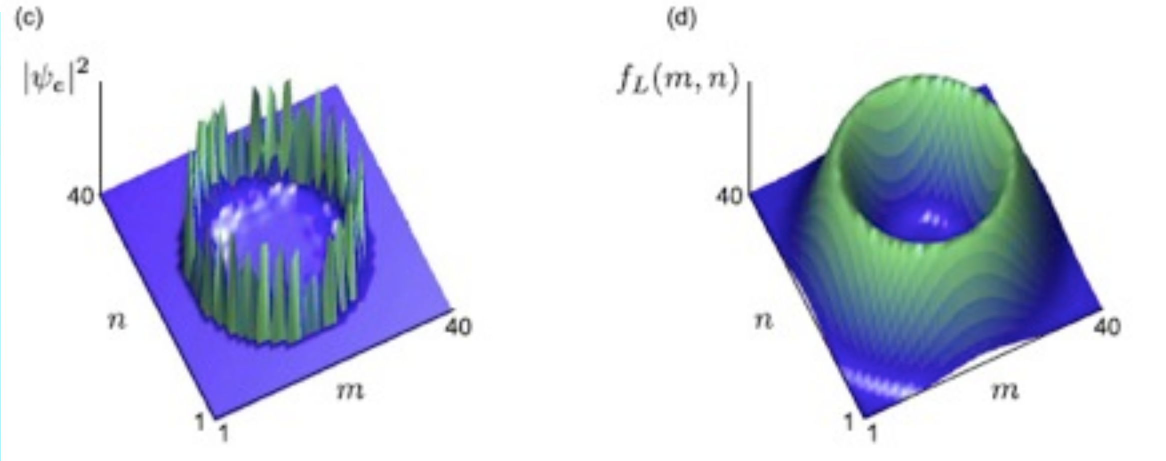
Detecting Chiral Edge States in the Hofstadter Optical Lattice

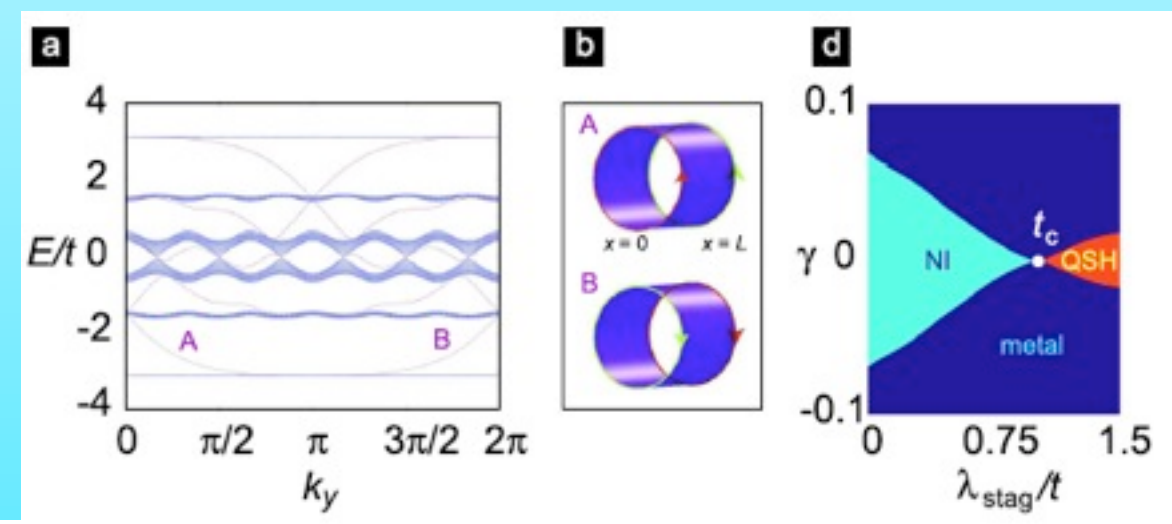
Nathan Goldman,[1,*] Jérôme Beugnon,[2] and Fabrice Gerbier[2]

[1]*Center for Nonlinear Phenomena and Complex Systems-Université Libre de Bruxelles (U.L.B.), B-1050 Brussels, Belgium*

[2]*Laboratoire Kastler Brossel, CNRS, ENS, UPMC, 24 rue Lhomond, 75005 Paris*

(Received 6 March 2012; published 19 June 2012)





PRL **105,** 255302 (2010) PHYSICAL REVIEW LETTERS week ending 17 DECEMBER 2010

Realistic Time-Reversal Invariant Topological Insulators with Neutral Atoms

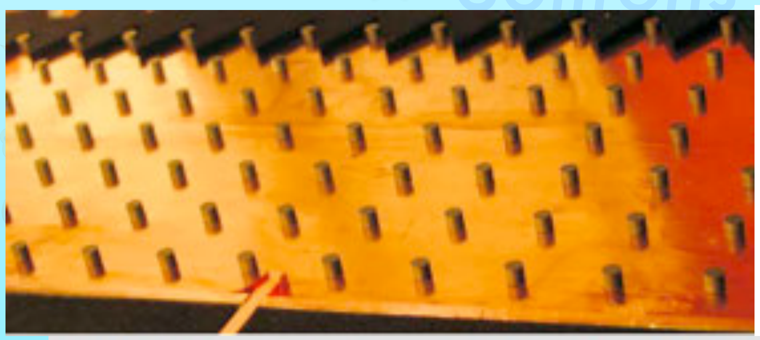
N. Goldman,[1] I. Satija,[2,3] P. Nikolic,[2,3] A. Bermudez,[4] M. A. Martin-Delgado,[4] M. Lewenstein,[5,6] and I. B. Spielman[7]

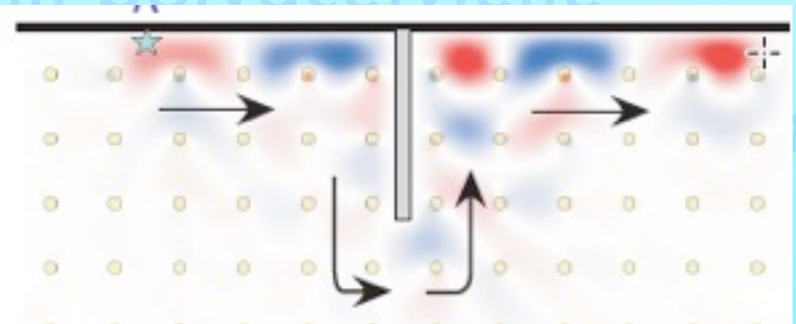
☆ One-way edge modes in gyromagnetic photonic crystals

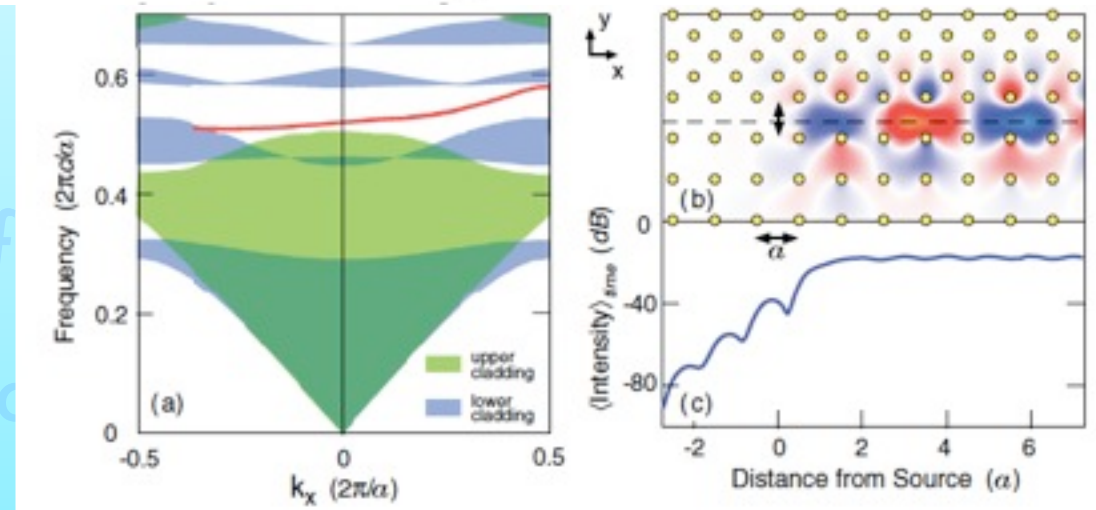
PRL 100, 013905 (2008) PHYSICAL REVIEW LETTERS week ending 11 JANUARY 2008

Reflection-Free One-Way Edge Modes in a Gyromagnetic Photonic Crystal

Zheng Wang, Y. D. Chong, John D. Joannopoulos, and Marin Soljačić







Vol 461 | 8 October 2009 | doi:10.1038/nature08293

Observation of unidirectional backscattering-immune topological electromagnetic states

Zheng Wang[1]*, Yidong Chong[1]†*, J. D. Joannopoulos[1] & Marin Soljačić[1]

PRL 100, 013904 (2008) PHYSICAL REVIEW LETTERS week ending 11 JANUARY 2008

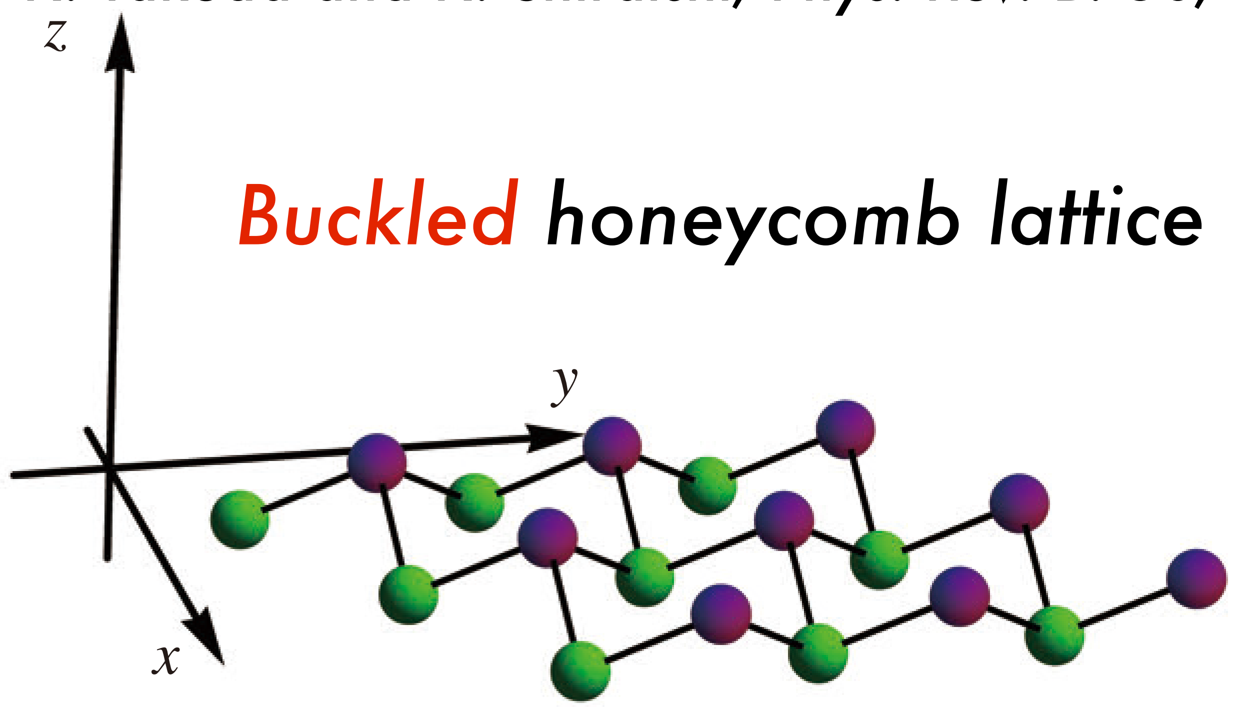
Possible Realization of Directional Optical Waveguides in Photonic Crystals with Broken Time-Reversal Symmetry

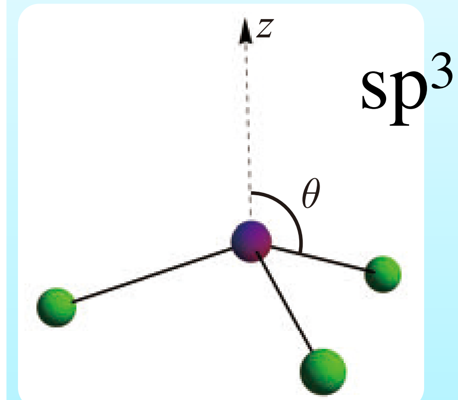
F. D. M. Haldane and S. Raghu*

Silicene : silicon analogue of graphene

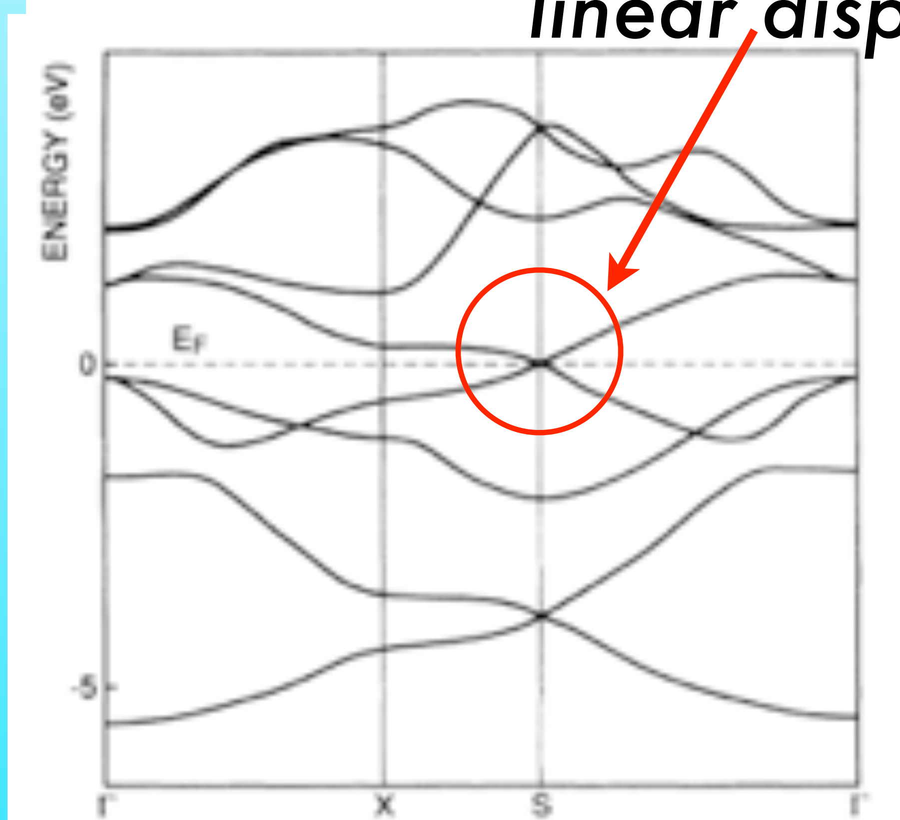
K. Takeda and K. Shiraishi, Phys. Rev. B. 50, 14916 (1994)

Buckled honeycomb lattice



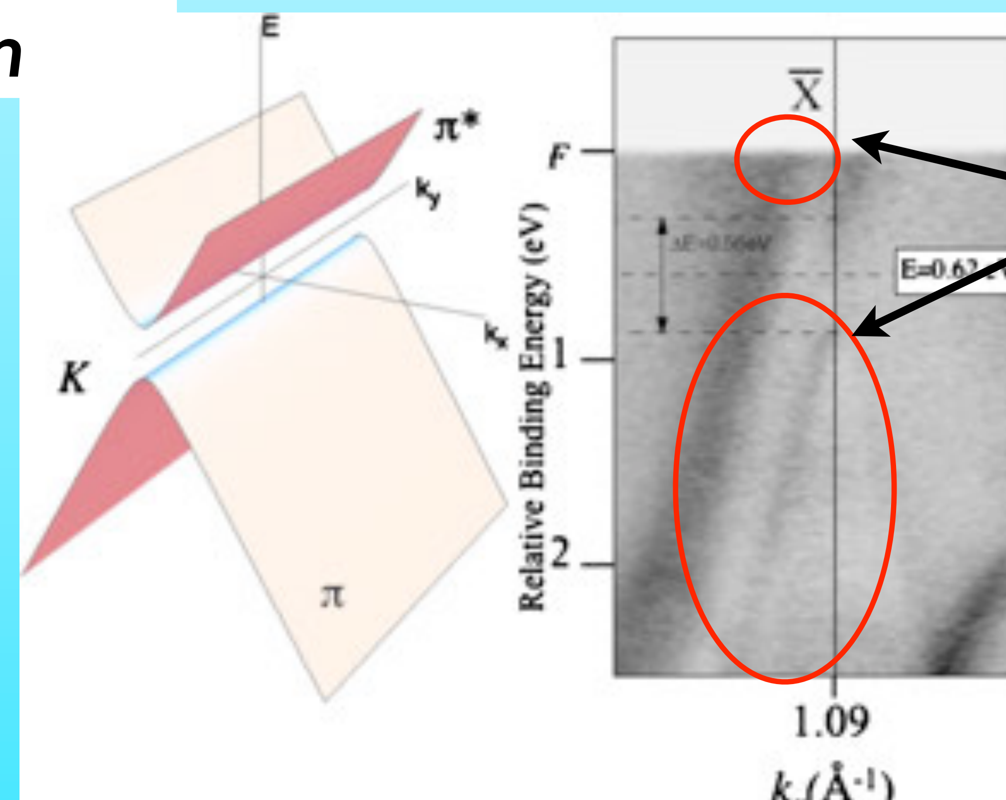


linear dispersion



Zero gap semiconductor

ARPES



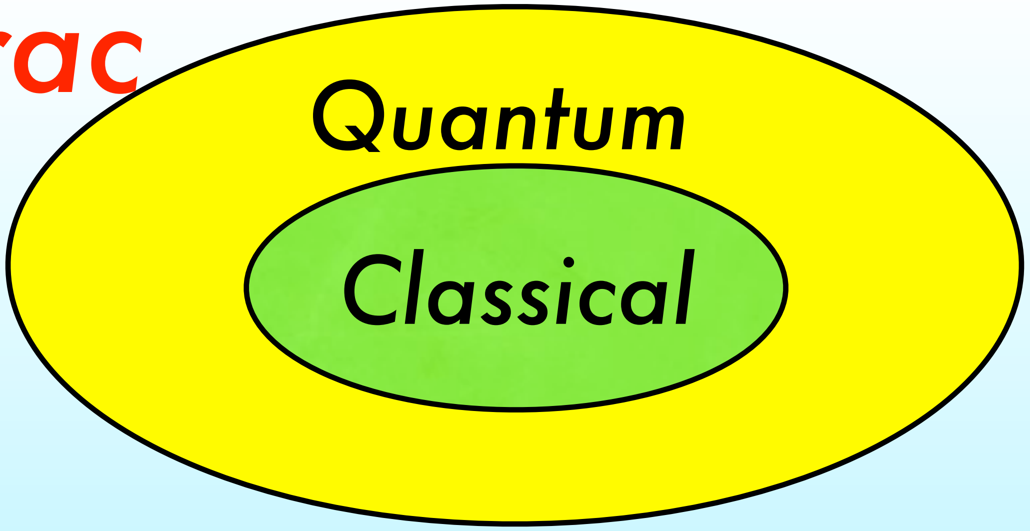
Dirac cone

P. D. Padova, et. el APL 96, (2010) 261905

Plan

- *Metal, insulator & semiconductor*
- *Bulk-edge correspondence :graphene, silicene and more*
- *From Newton to Dirac for devices breakthrough*

From Newton to Dirac



☆ Classical & Quantum

M. Planck ~1900

The Munich physics professor Philipp von Jolly advised Planck against going into physics, saying, "in this field, almost everything is already discovered, and all that remains is to fill a few holes."

Wrong ! Quantum mechanics & Relativity

Newton (classical) → Dirac (quantum & relativistic)

Crossover : No clear boundaries

Future devices: Breakthrough by quantum effects

Quantum computer may be too hard

From Newton to Dirac

☆ Classical & Quantum

Future devices: Breakthrough by quantum effects

☆ Planck定数：唯一の量子論固有の定数

$\hbar$ = 6.626068 × 10^{-34} [J・s]

[J・s] = （エネルギー）×（時間）=（運動量）×（長さ）= (角運動量)

= [kg・m/s^2・m・s]= [kg・m/s・m]

（エネルギー）×（時間）
（運動量）×（長さ）
(角運動量)
} >> $\hbar$：classical
≈ $\hbar$：quantum

$\hbar$/10[nm]= p=6.6 × 10^{-26}[kg・m/s], $p^2/2m_e$=0.015[eV]

$\hbar$/10[fs]= E=6.6 × 10^{-20}[J]=0.4[eV]

electron spin = $\hbar/2$ ：purely quantum

From Newton to Dirac

What's spin ?　　Non-relativistic limit of the Dirac hamiltonian

$H =$

Spin ← Quantum mechanics + Relativity

Spin: natural inner degree of freedom　　relativistic correction

$$H\psi = \psi E \qquad \psi = \begin{bmatrix} \psi_\uparrow \\ \psi_\downarrow \end{bmatrix}$$ spinor

charge $\rho = |\psi|^2,\ j = -i\hbar\psi^\dagger\nabla\psi + h.c.$

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\, j = 0$$ conserve

spin $\rho_S = \psi^\dagger\sigma\psi,\ j_S = -i\hbar\psi^\dagger\sigma\nabla\psi + h.c.$

$$S^+ = \psi_\uparrow^\dagger\psi_\downarrow \qquad S^- = \psi_\downarrow^\dagger\psi_\uparrow$$

$$\frac{\partial \rho_S}{\partial t} + \mathrm{div}\, j_S \neq 0$$ does not conserve

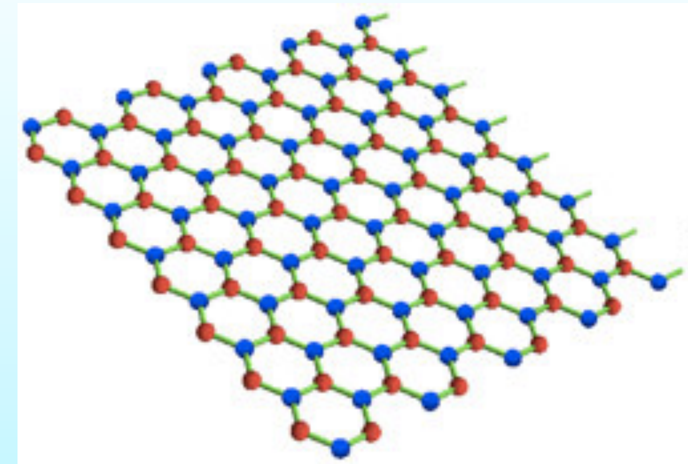
Time reversal　$\boldsymbol{S} \to -\boldsymbol{S}$

spin breaks TR
spinor is OK　: Kramers degeneracy:

One more half electrons

1. Zero gap semiconductors

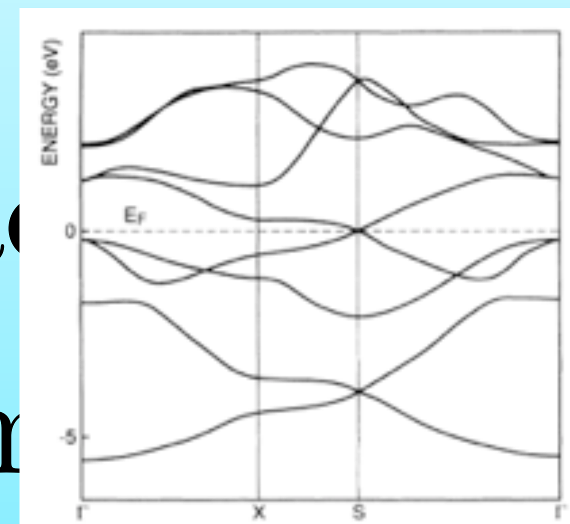
$$H_{zero} = \pm\sqrt{H_{ele}}$$

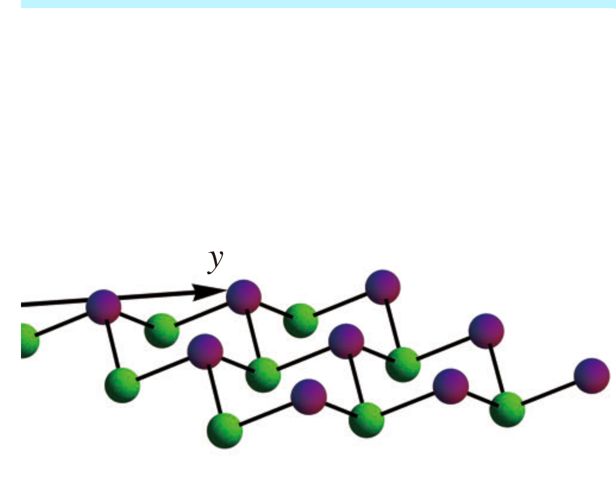


2. Majorana fermions

$$H_{Majo,R} = \mathrm{Re}$$

$$H_{Majo,I} = \mathrm{Im}$$





$$H_{ele} = H_{Majo,R} + iH_{Majo,I}$$

Breakthrough of the Year, 2012

Science AAAS

Science 25 May 2012:
Vol. 336 no. 6084 pp. 1003-1007

Signatures of Majorana Fermions in Hybrid Superconductor-Semiconductor Nanowire Devices

V. Mourik[1,*], K. Zuo[1,*], S. M. Frolov[1], S. R. Plissard[2], E. P. A. M. Bakkers[1,2], L. P. Kouwenhoven[1,†]

Conclusion

Quantum effects are everywhere
in
condensed matter physics

Use of the Quantum effects
in quantum nano devices