What is a topological insulator?

Jennifer Cano

Stony Brook University

FLATIRON INSTITUTE

NSF

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
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Fundamental goal of condensed matter physics: understand phases of matter

Solid

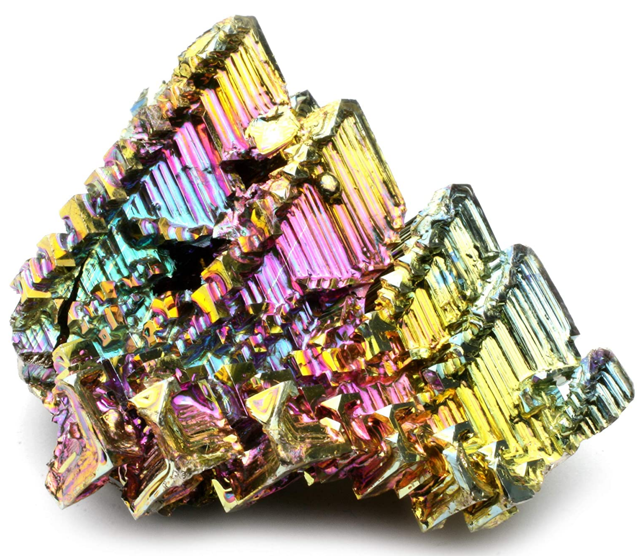
Liquid

Gas

How are atoms arranged?

Fundamental goal of condensed matter physics: understand phases of matter

Metal

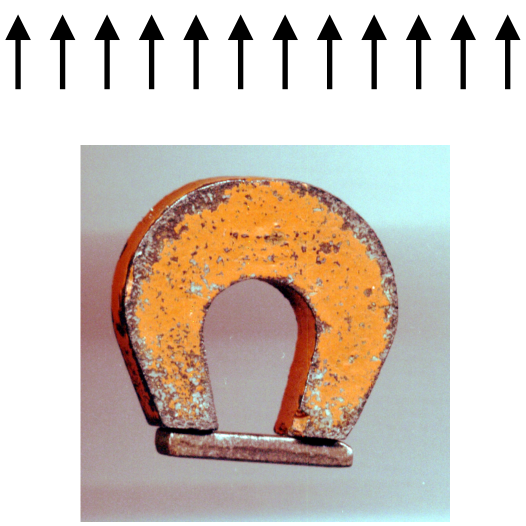


Insulator

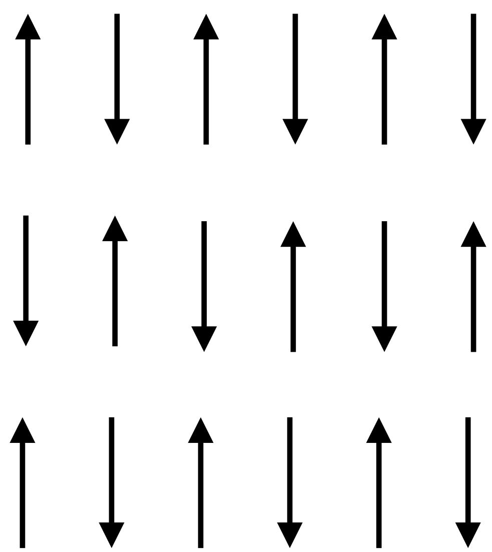
How are electrons arranged?

Fundamental goal of condensed matter physics: understand phases of matter

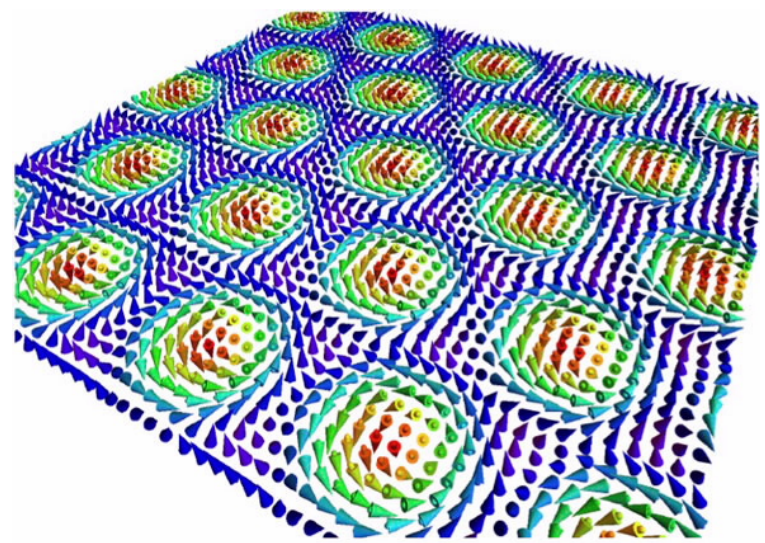
Ferromagnet



Antiferromagnet

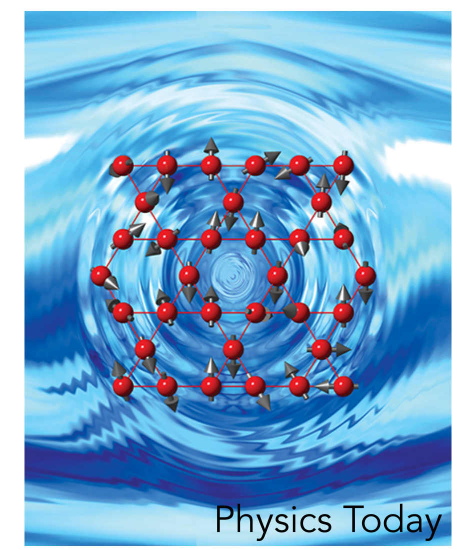


Skyrmion lattice



MnSi: phys.org

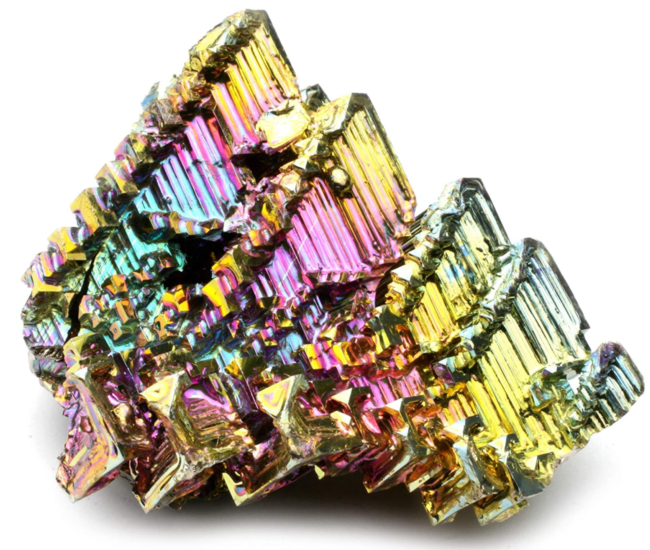
Quantum spin liquid

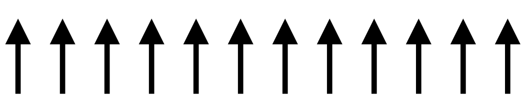


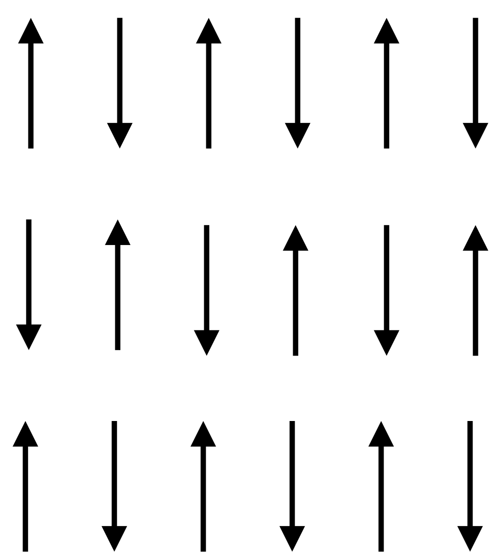
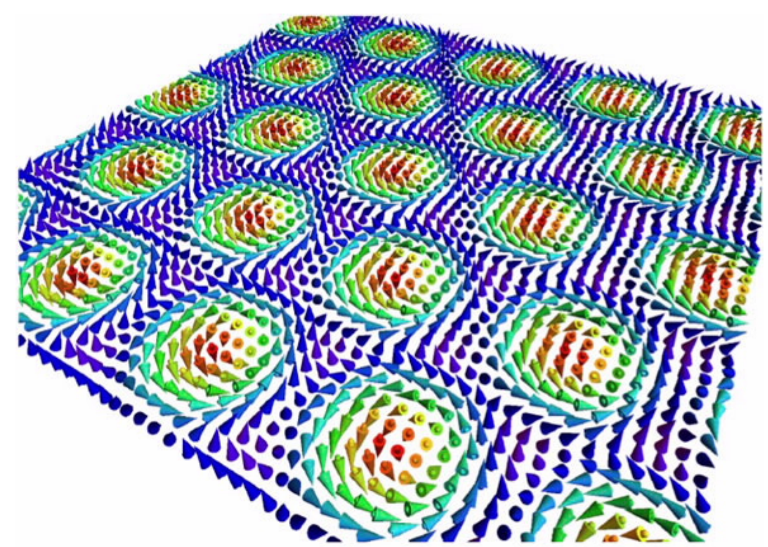
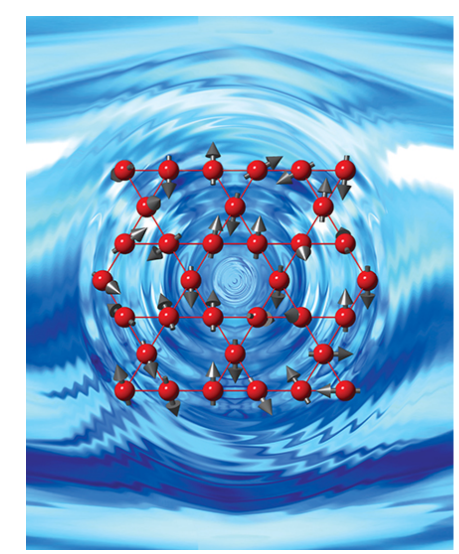
How are electron spins arranged?

What’s in a crystal? A quantum universe



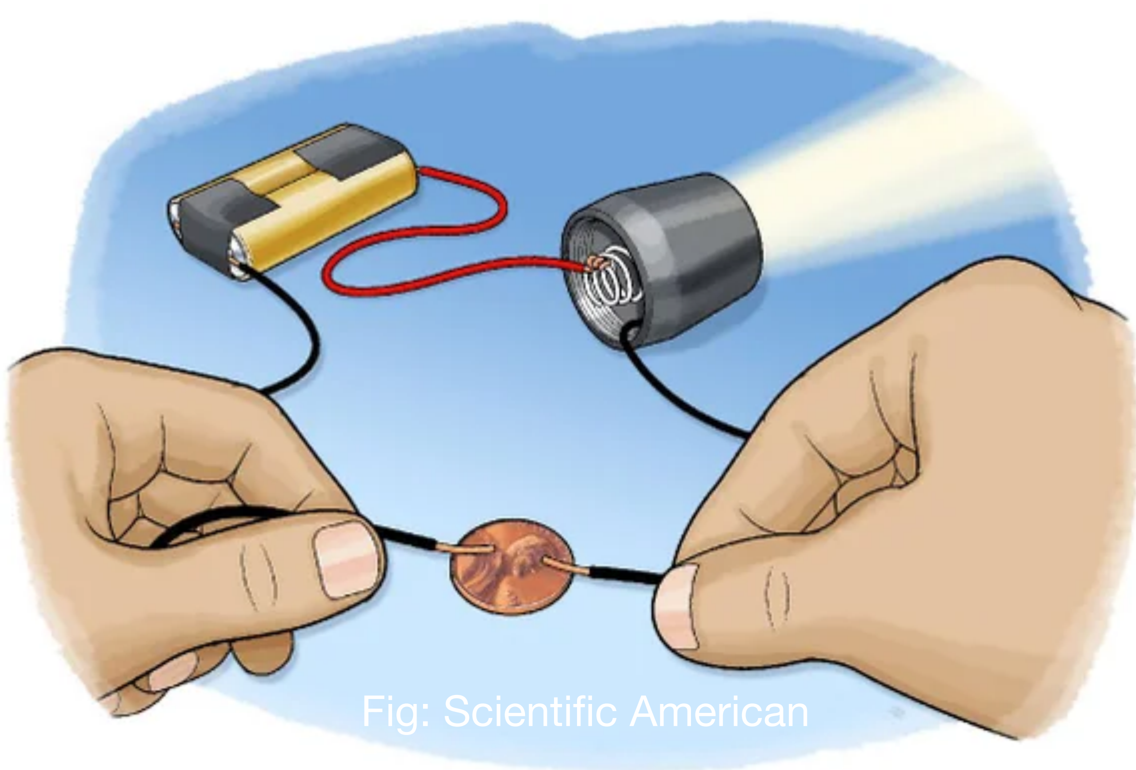





Metal vs insulator

Metals conduct electricity



Insulators resist it

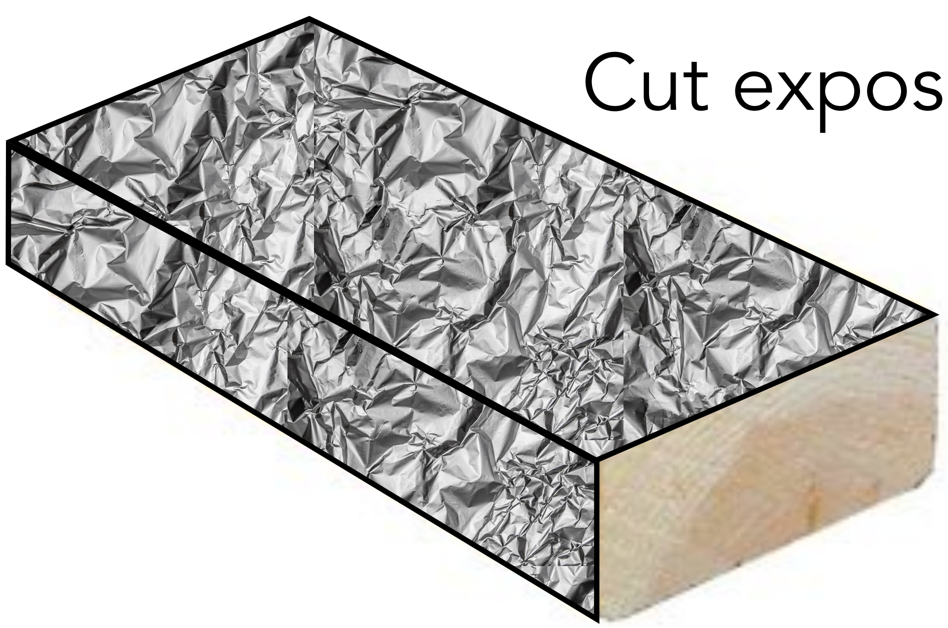
"Topological" insulators:

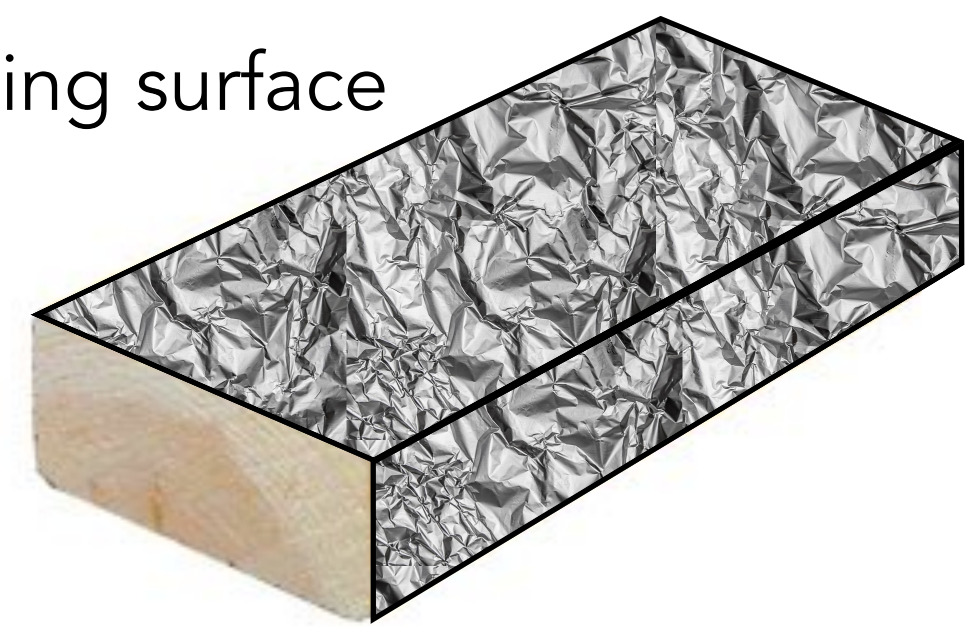
insulating in bulk but metallic on surface

Can you make one at home? e.g., wrap a wood block in tin foil

NO!

Cut exposes insulating surface





“Topological” insulators:

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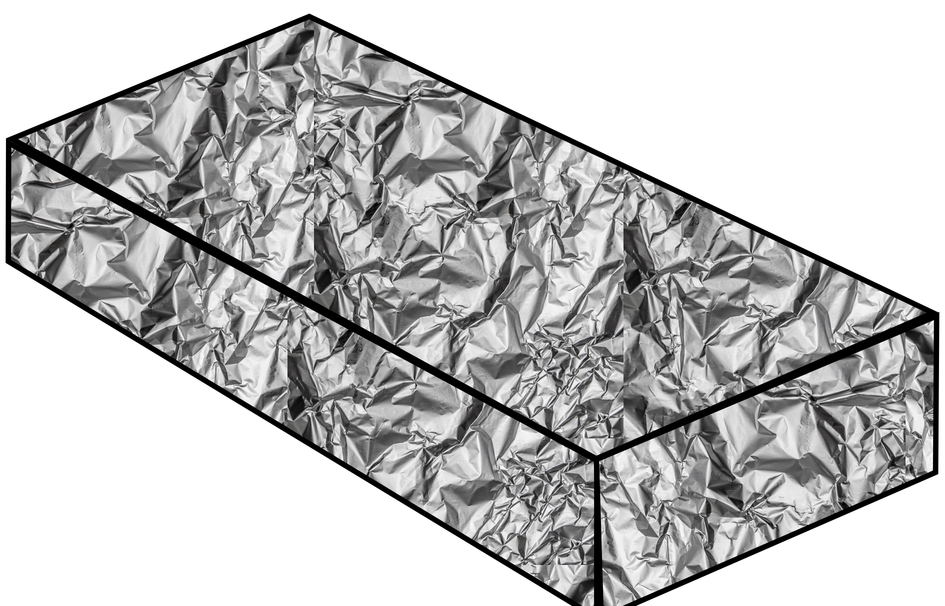
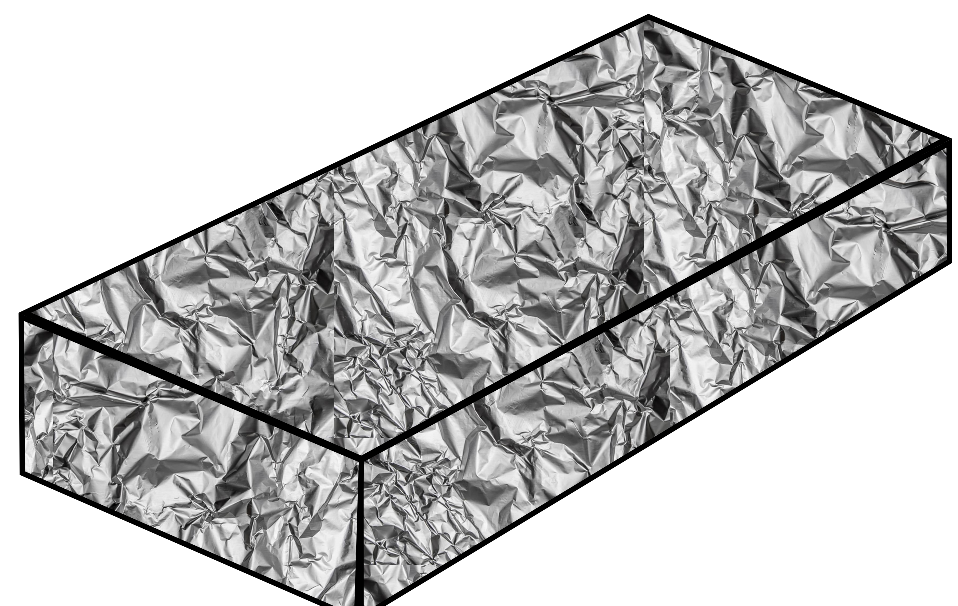
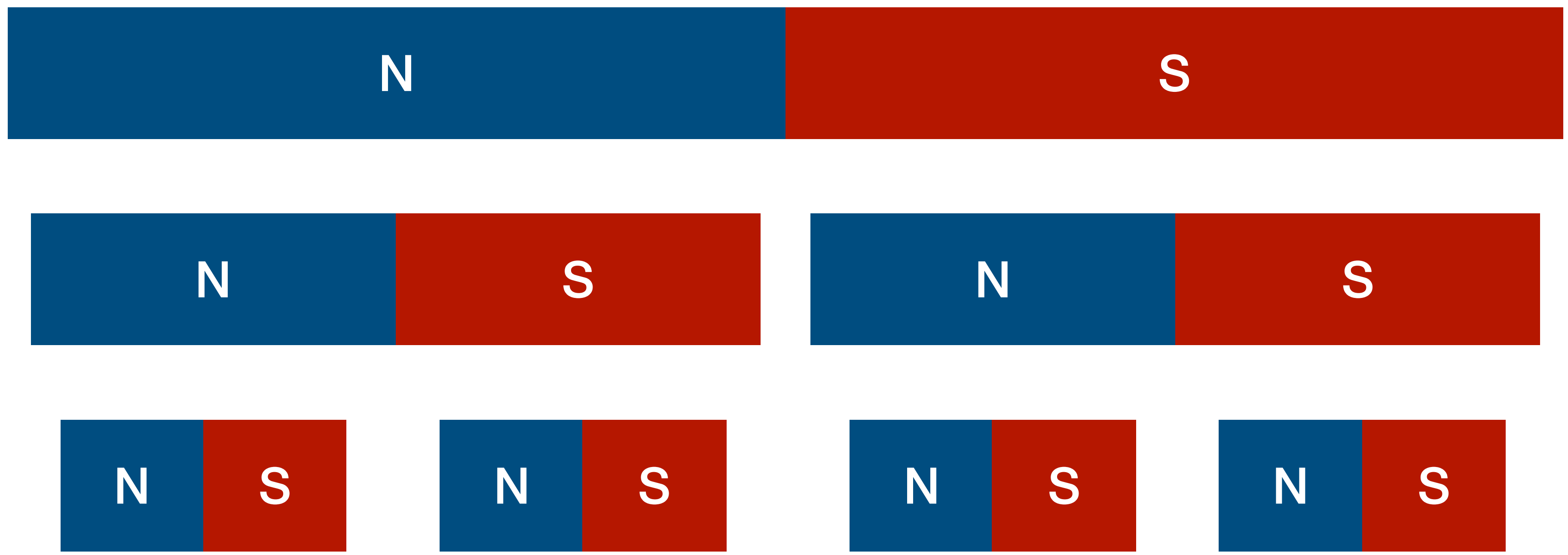
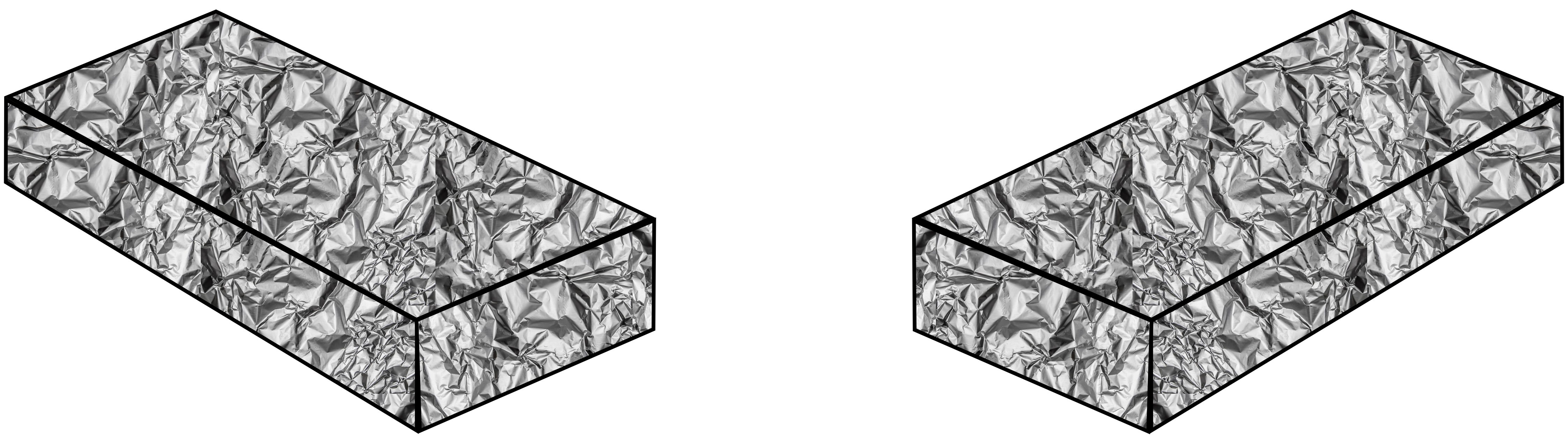




All surfaces of a topological insulator are conducting

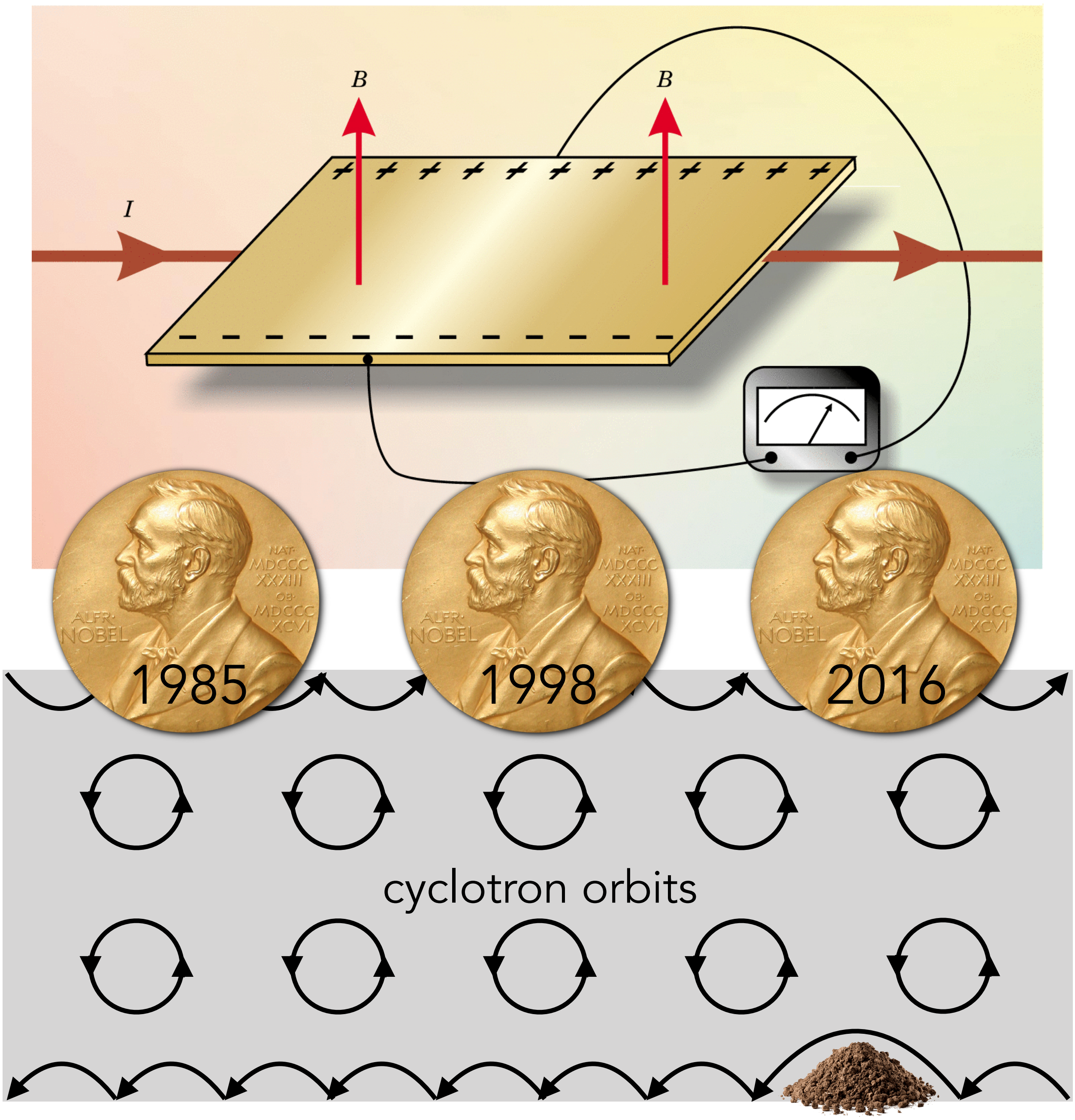
“Topological” insulators:
insulating in bulk but metallic on surface





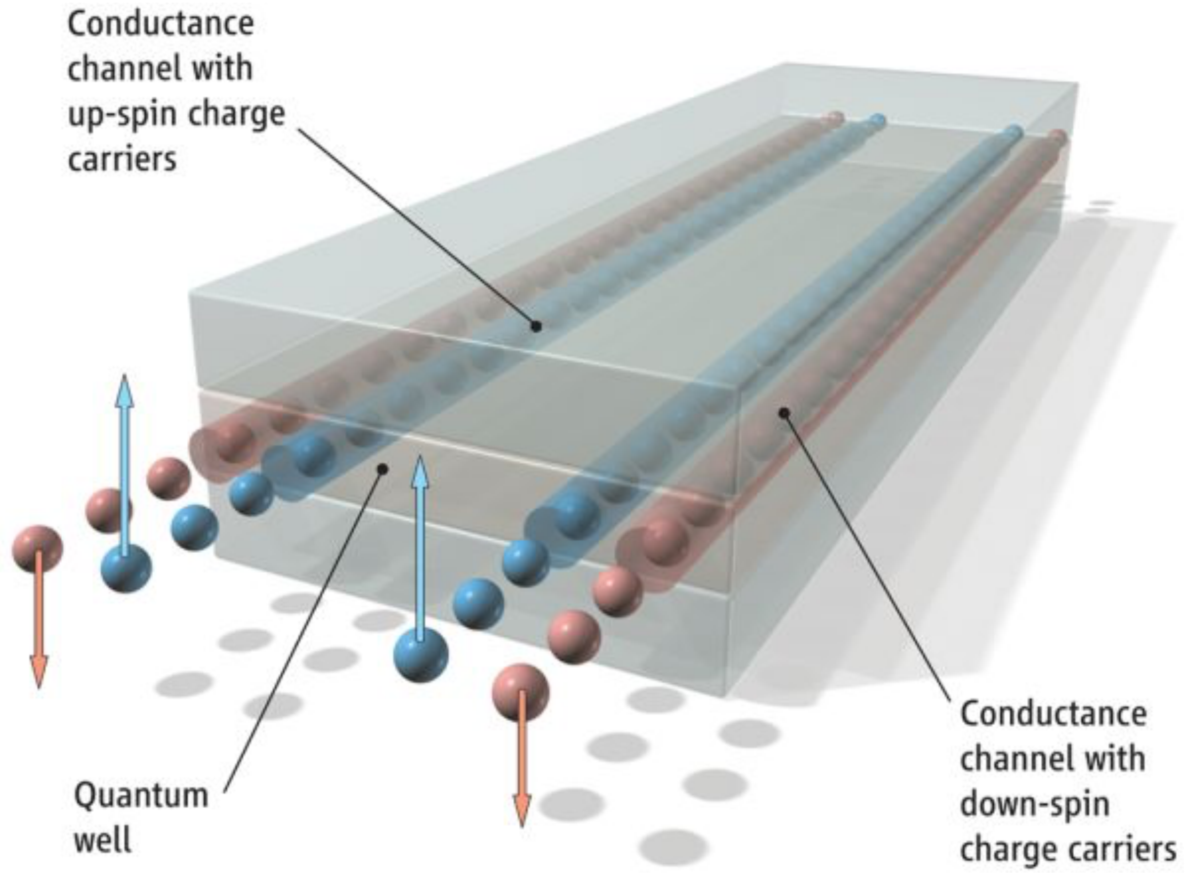
All surfaces of a topological insulator are conducting

2D example: "quantum Hall effect"



Current moves in one direction

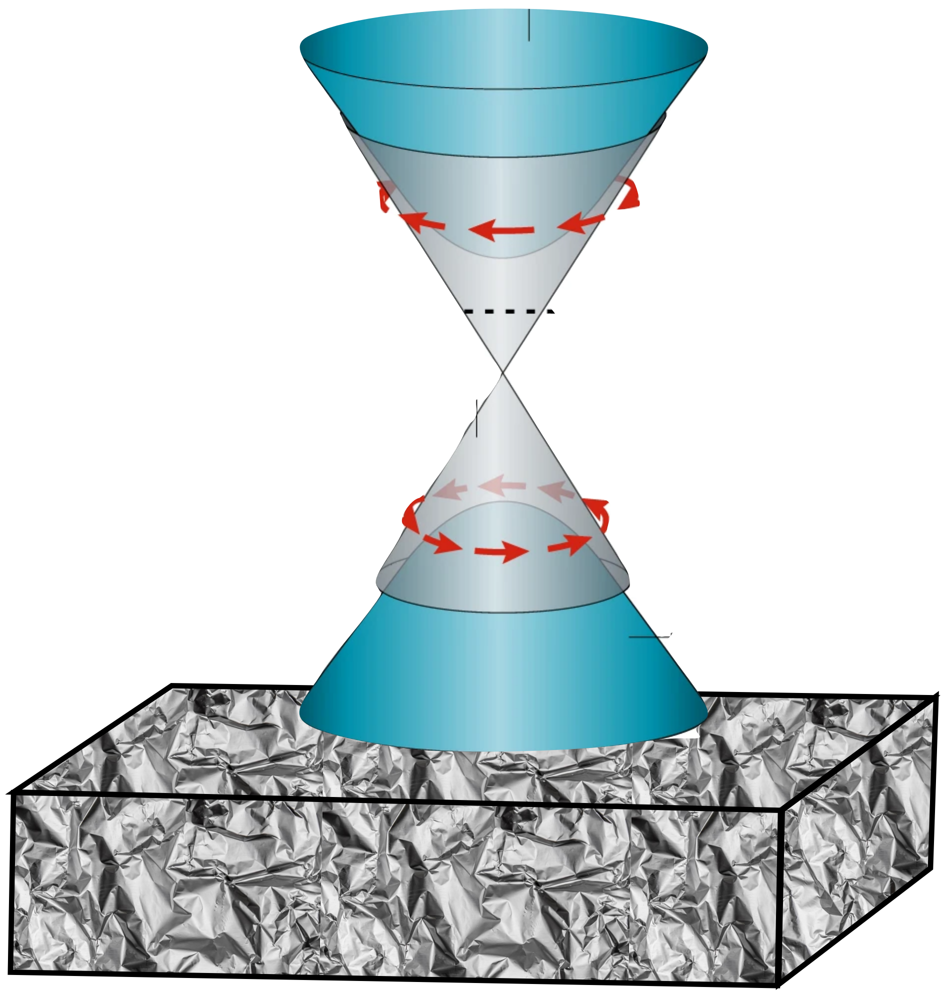
2D example: "quantum ^spin Hall effect"



Autobahn for electron spins

Electron spin current in opposite directions

3D topological insulator

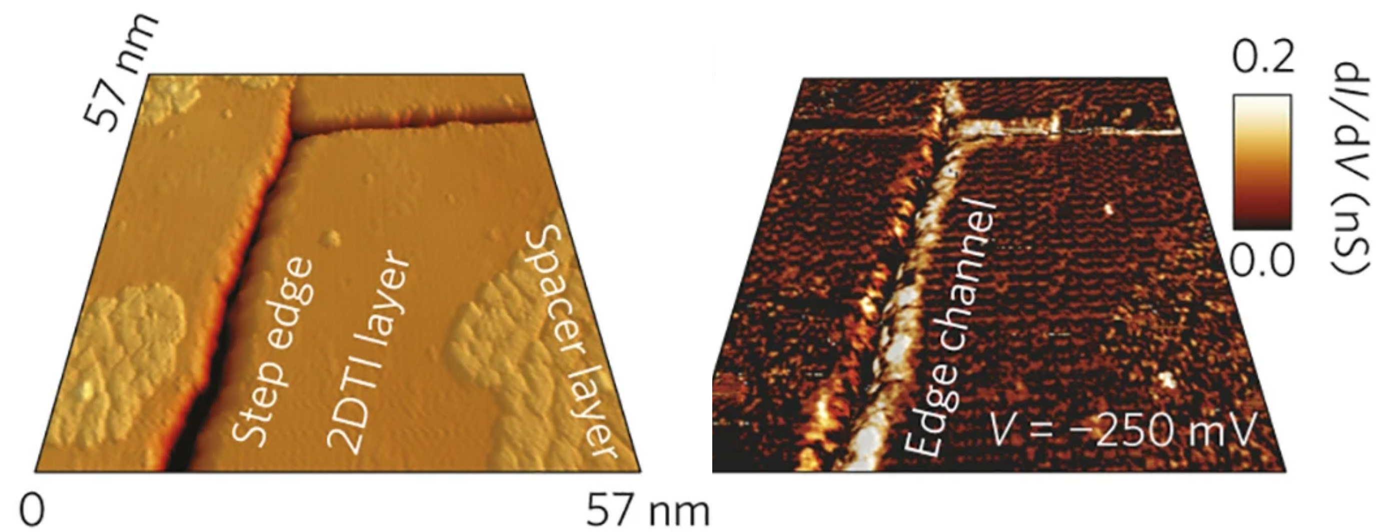


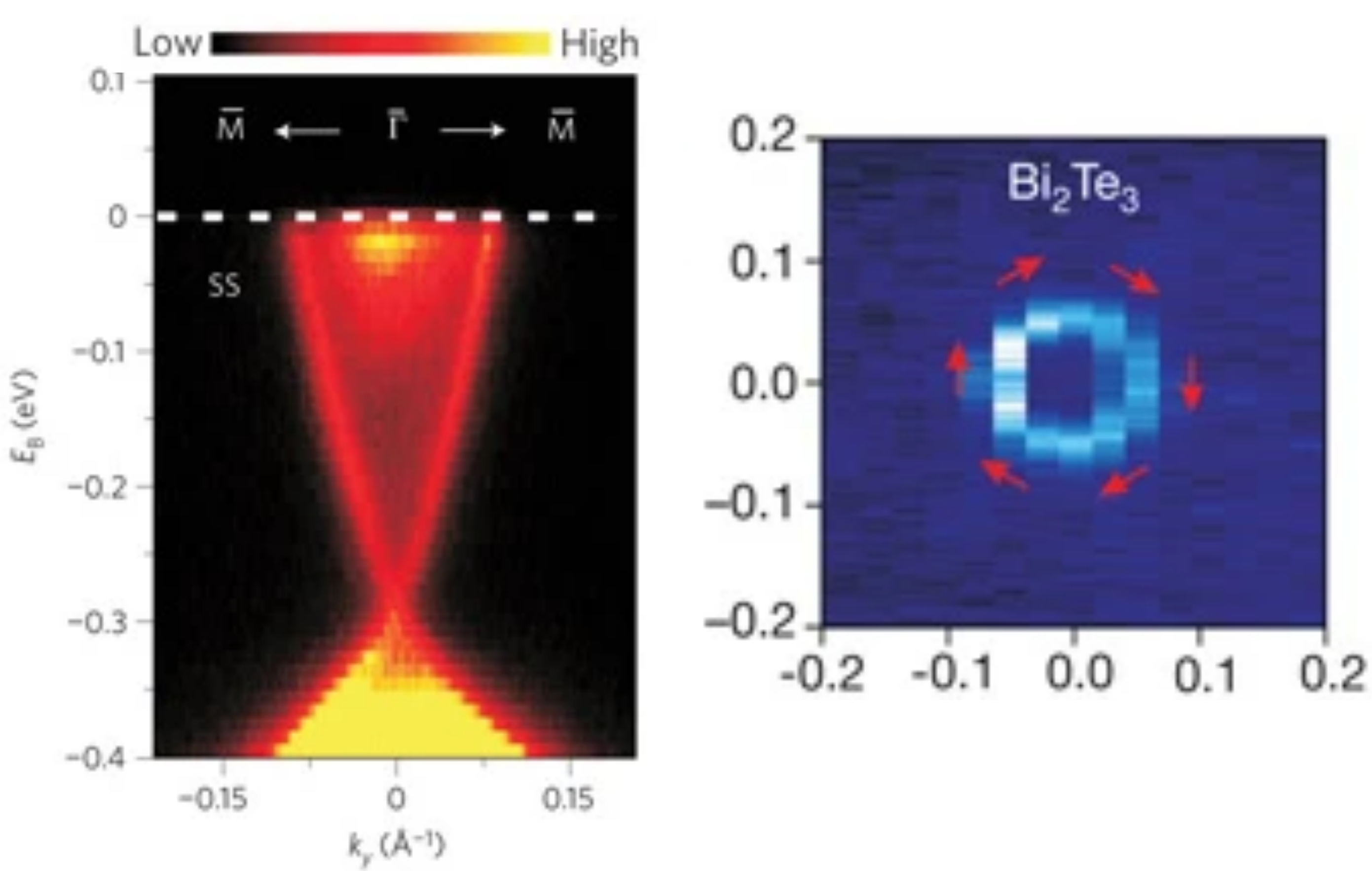
“Spin-momentum locking”

Measurements of topological surface states

2D: Scanning tunneling microscopy $Bi_{14}Rh_3I_9$

Pauly et al Nat. Phys. 11, 338-343 (2015)



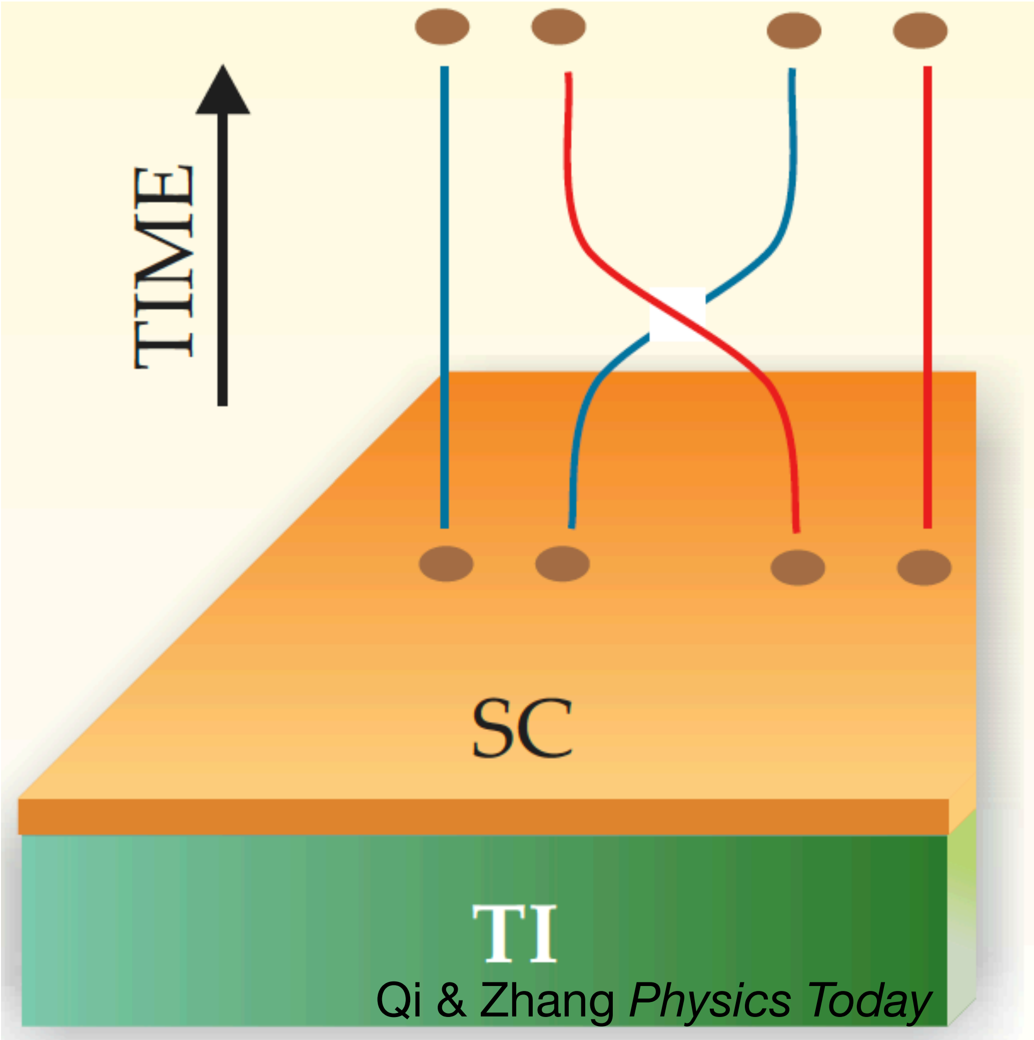


3D: Angle resolved photoemission spectroscopy Bi_2Te_3

Xia et al Nat. Phys. 5, 398-402 (2009)
Hsieh et al Nature 460, 1101-1105 (2009)

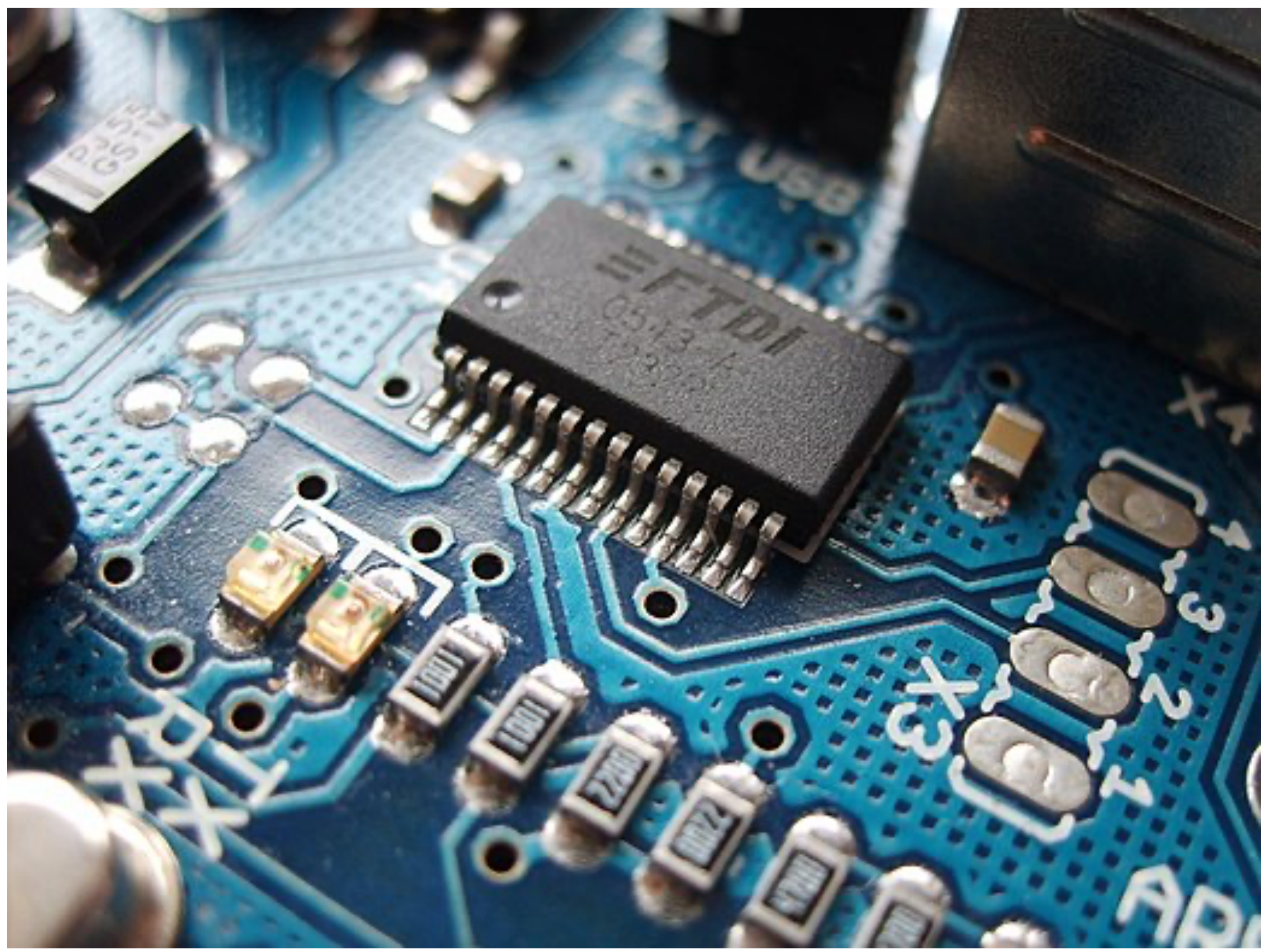
Why do we care about topological insulators?

Application: quantum computing

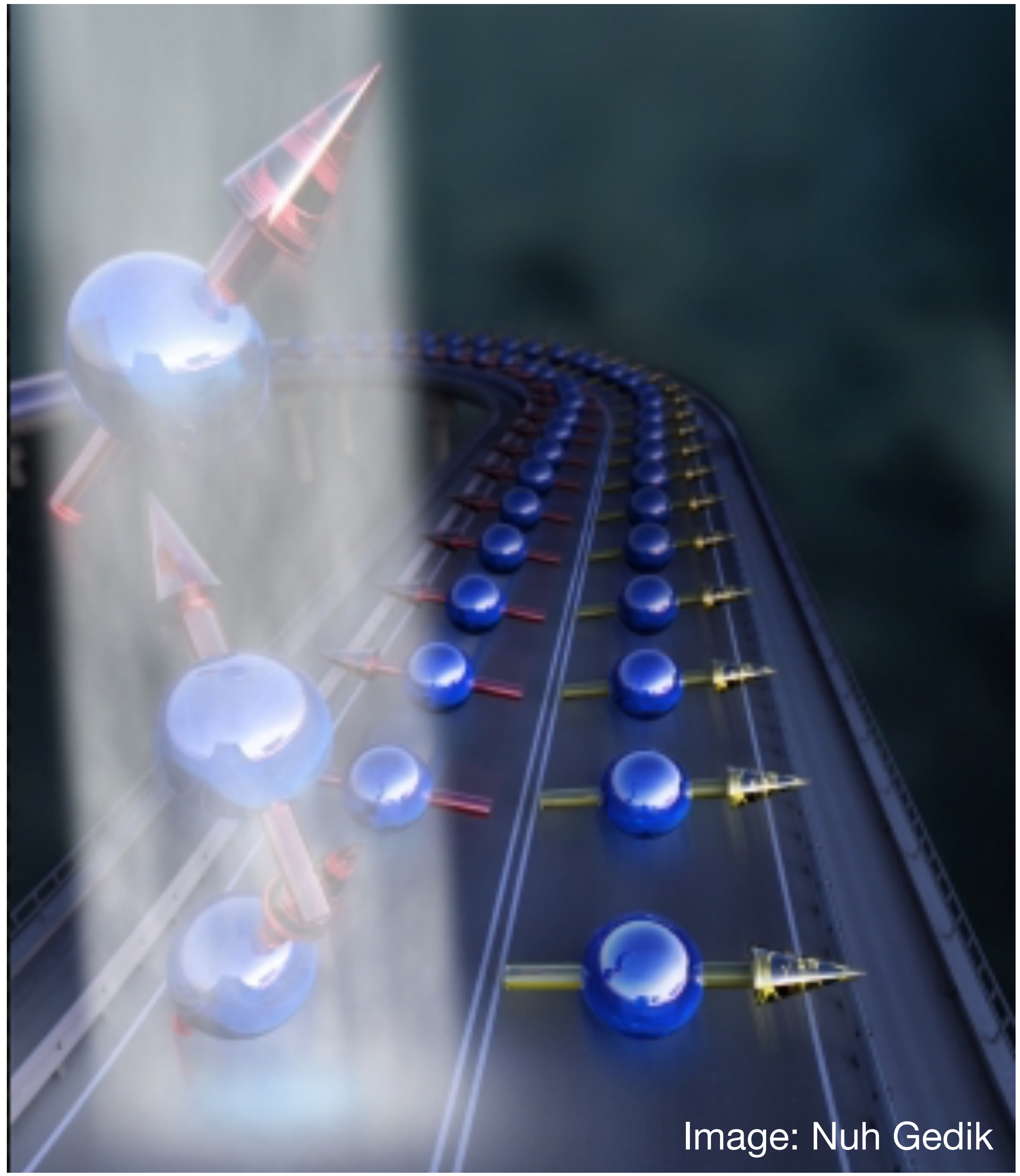


Qi & Zhang *Physics Today*

Application:
energy-efficient electronics



Application: spintronics



Theory of topological insulators: outline

1. Electronic band structure:

— orbitals and hybridization

— metal vs insulator

2. What is topology?

3. How to apply topology to band structure?

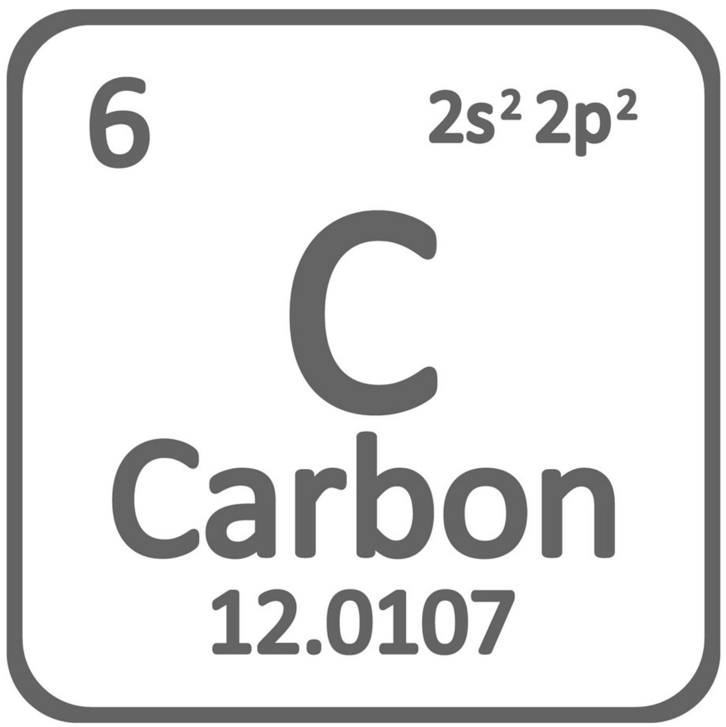
4. Flavor of current research directions

What is a band structure?

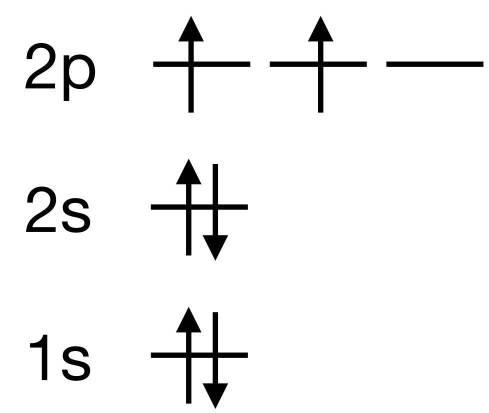
Atomic orbitals:
electron energy levels on a single atom

	s ($\ell = 0$)	p ($\ell = 1$)			d ($\ell = 2$)					f ($\ell = 3$)						
	$m = 0$	$m = 0$	$m = \pm1$		$m = 0$	$m = \pm1$		$m = \pm2$		$m = 0$	$m = \pm1$		$m = \pm2$		$m = \pm3$	
	s	p_z	p_x	p_y	d_{z^2}	d_{xz}	d_{yz}	d_{xy}	$d_{x^2-y^2}$	f_{z^3}	f_{xz^2}	f_{yz^2}	f_{xyz}	$f_{z(x^2-y^2)}$	$f_{x(x^2-3y^2)}$	$f_{y(3x^2-y^2)}$
$n = 1$																
$n = 2$																
$n = 3$																
$n = 4$																
$n = 5$										. . .	. . .	. . .	. . .	. . .	. . .	. . .
$n = 6$					. . . ‡	. . .	. . . ‡	. . .	. . . ‡	. . . *	. . . *	. . . *	. . . *	. . . *	. . . *	. . . *
$n = 7$		. . . †	. . . †	. . . †	. . . *	. . . *	. . . *	. . . *	. . . *	. . . *	. . . *	. . . *	. . . *	. . . *	. . . *	. . . *

Atomic orbitals:
electron energy levels on a single atom



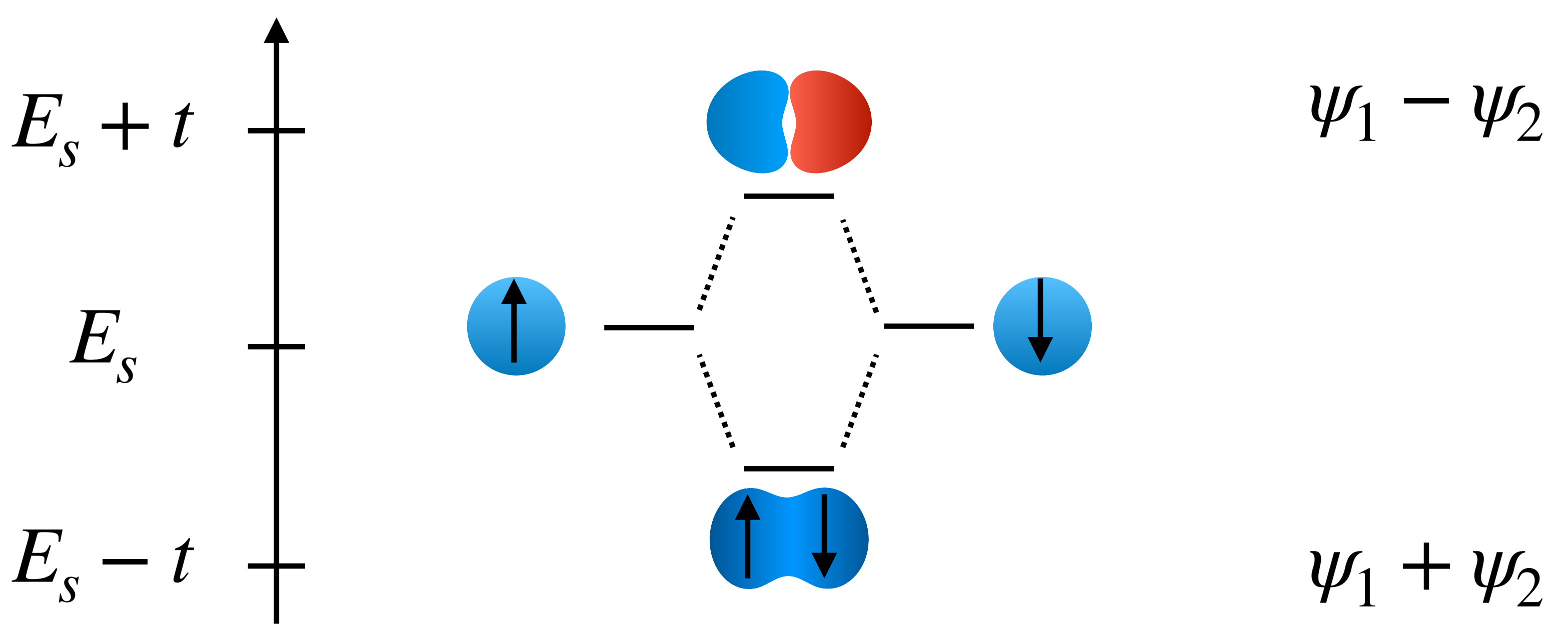
Ex: Carbon



Two spins per energy level

Electron bonding: electron energy levels on two atoms

Orbitals from two atoms hybridize to save energy

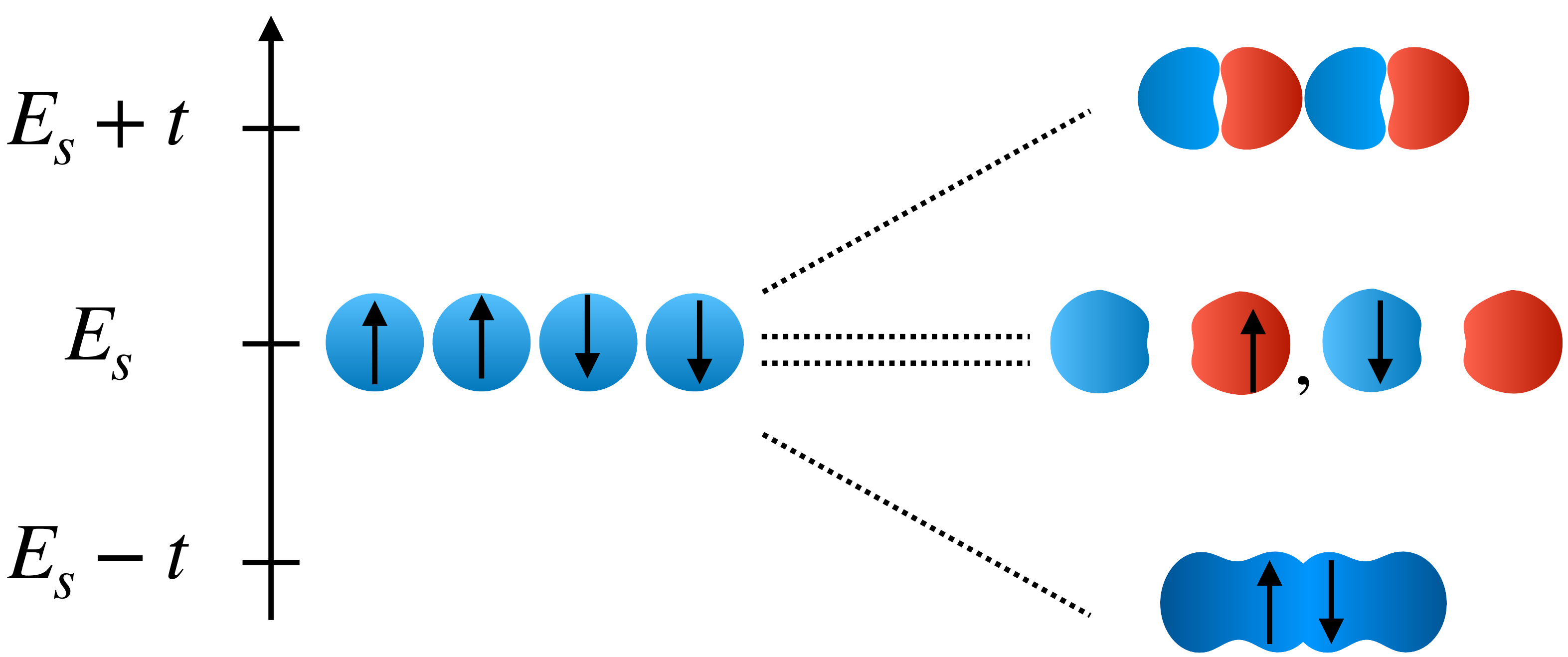


<u>Total energy:</u>

Not hybridized: $2E_s$ Hybridized: $2E_s - 2t$

Electron bonding: electron energy levels on four atoms

Orbitals from more atoms form more hybridized states



$$\psi_1 - \psi_2 + \psi_3 - \psi_4$$

$$\psi_1 - \psi_3,\ \psi_2 - \psi_4$$

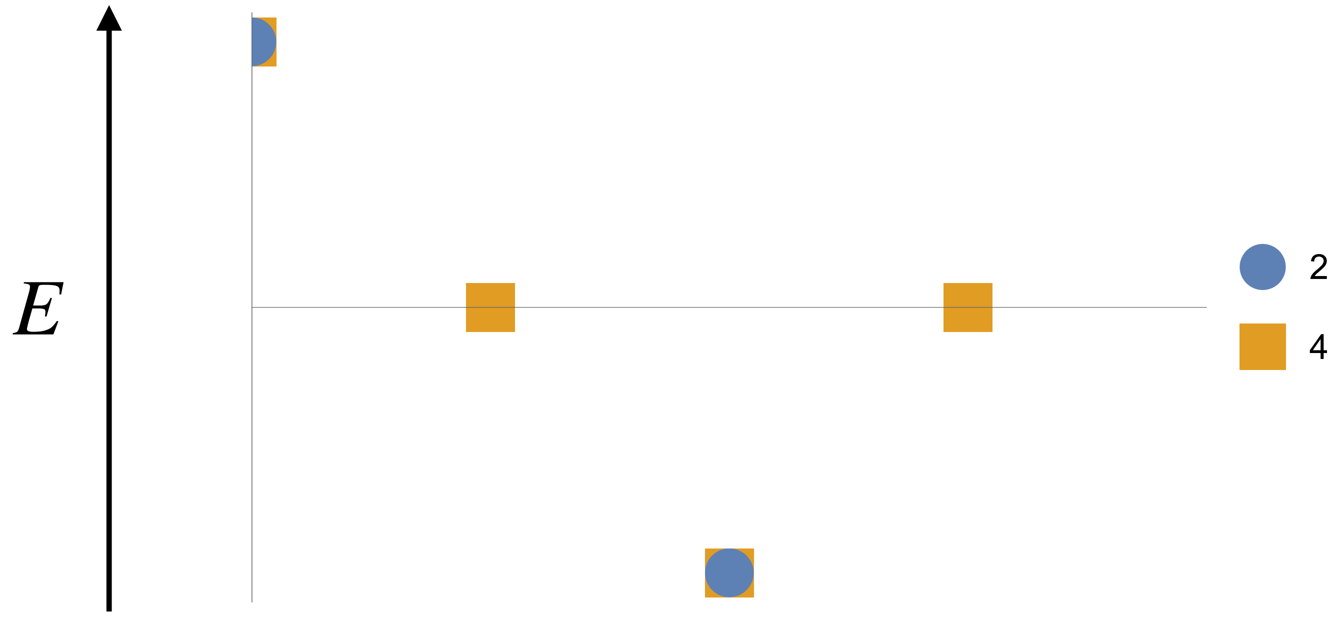
$$\psi_1 + \psi_2 + \psi_3 + \psi_4$$

Total energy:

Not hybridized: $4E_s$ Hybridized: $4E_s - 2t$

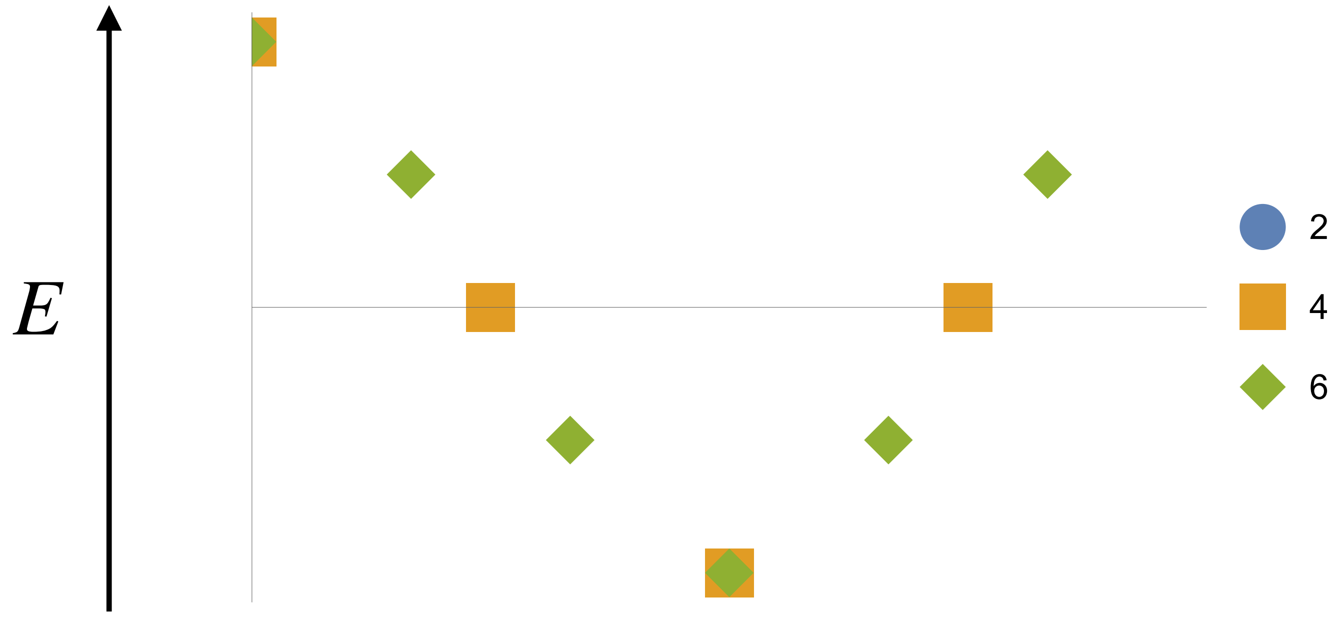
Electron bonding:
Plot electron energy levels on multiple atoms

2, 4 atoms



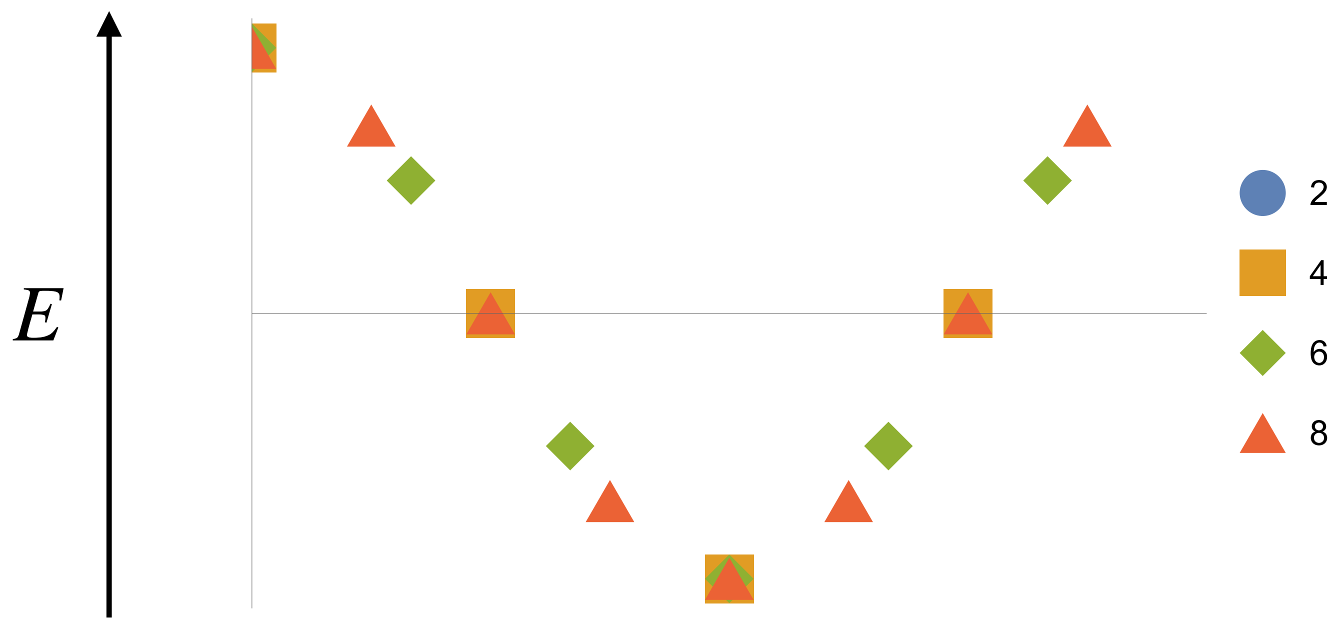
Electron bonding:
Plot electron energy levels on multiple atoms

2, 4, 6 atoms



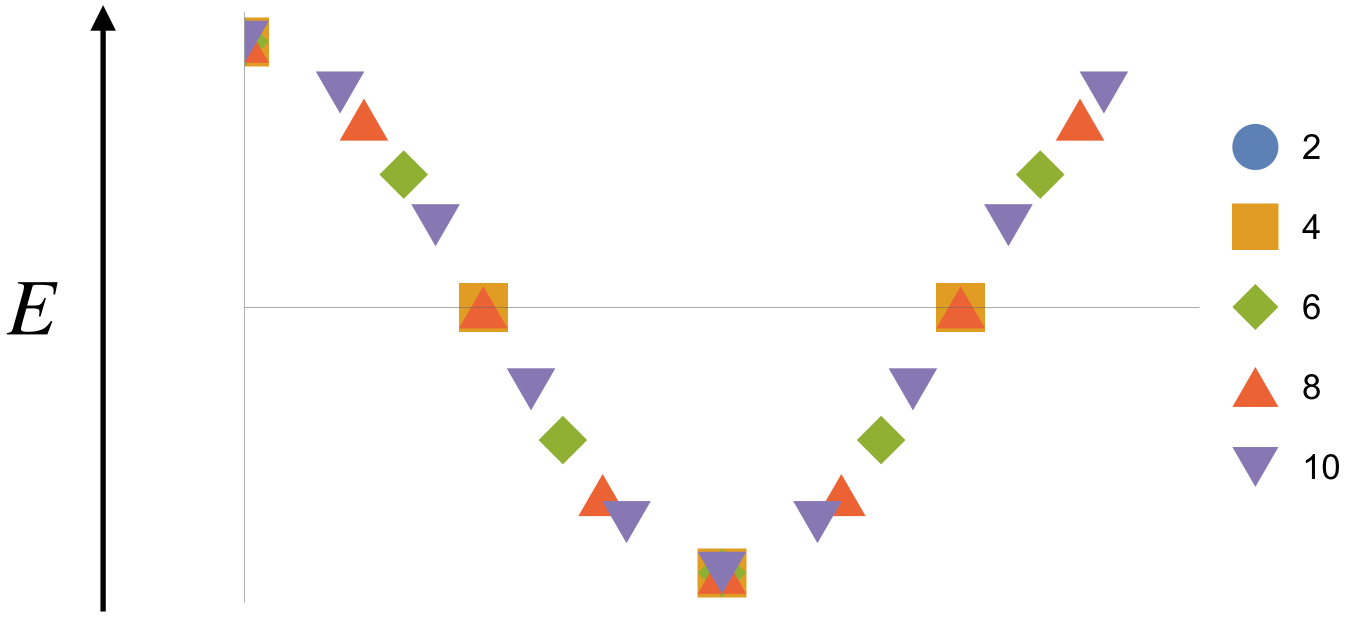
Electron bonding:
Plot electron energy levels on multiple atoms

2, 4, 6, 8 atoms



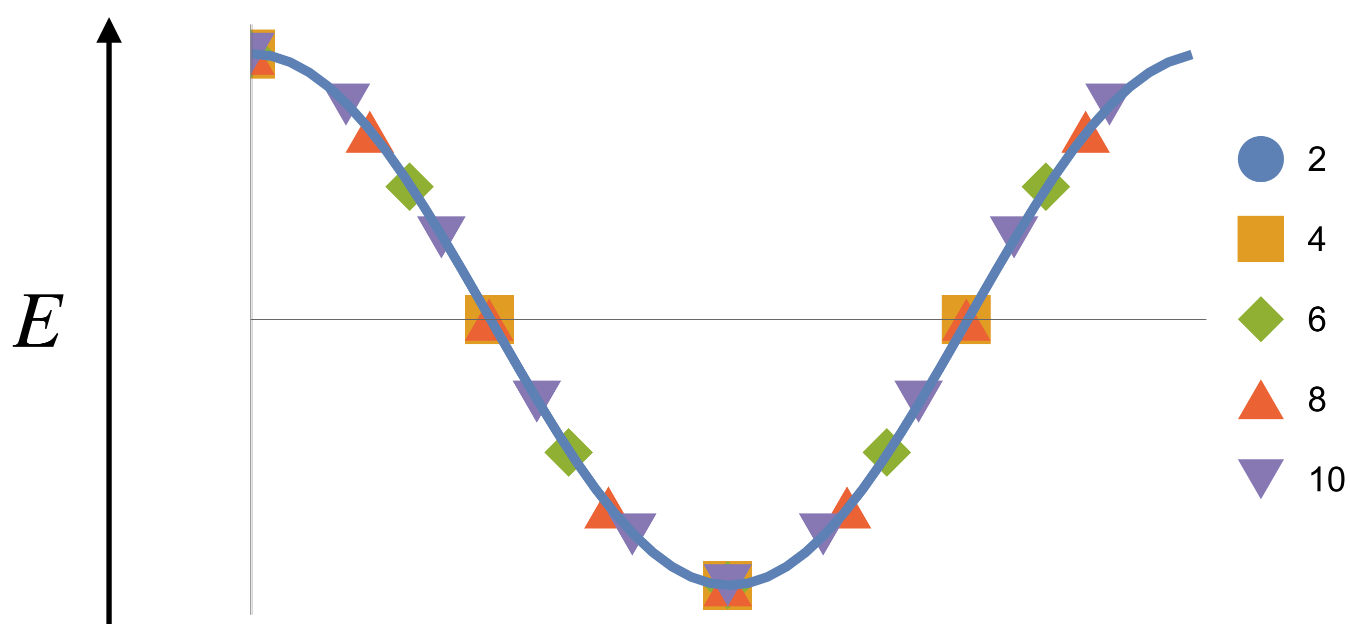
Electron bonding:
Plot electron energy levels on multiple atoms

2, 4, 6, 8, 10 atoms

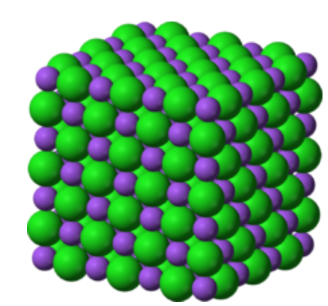


Electron bonding:
Plot electron energy levels on multiple atoms

2, 4, 6, 8, 10 atoms → points fall on a cosine curve



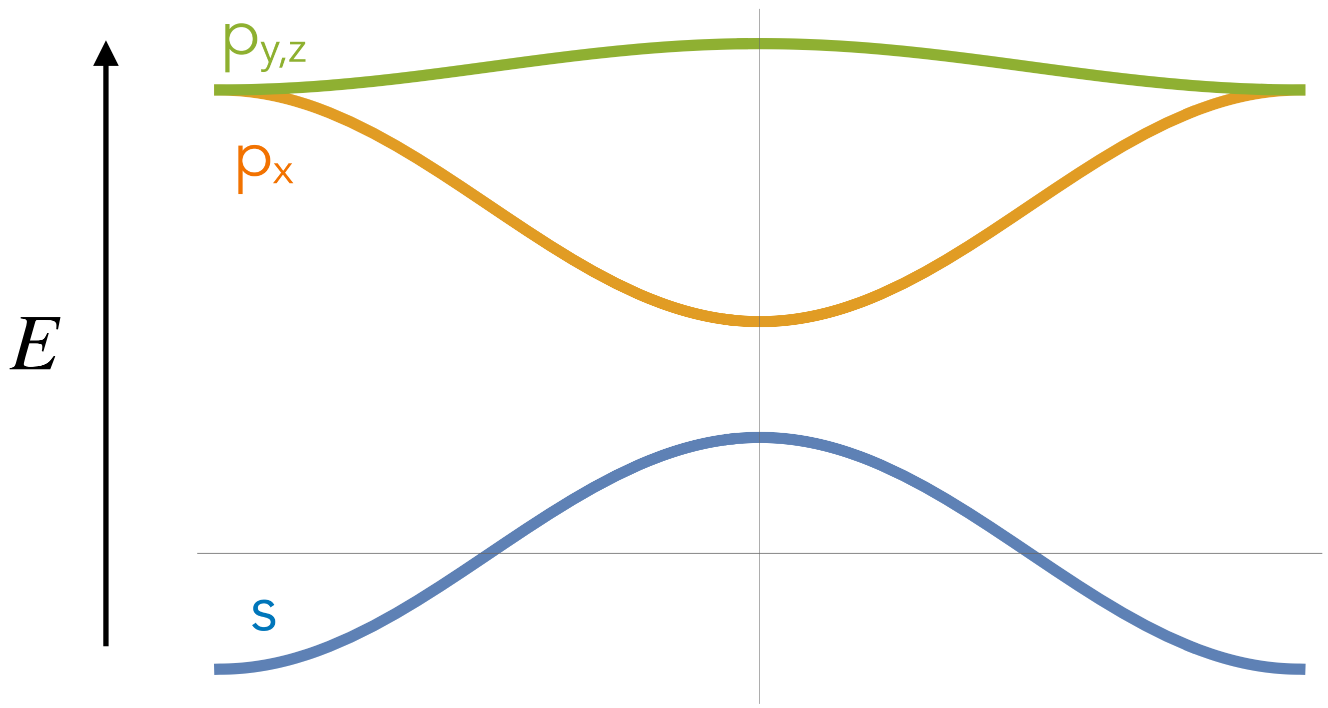
$$E(k) = -\, t\cos(ka), k = 2\pi n/Na$$



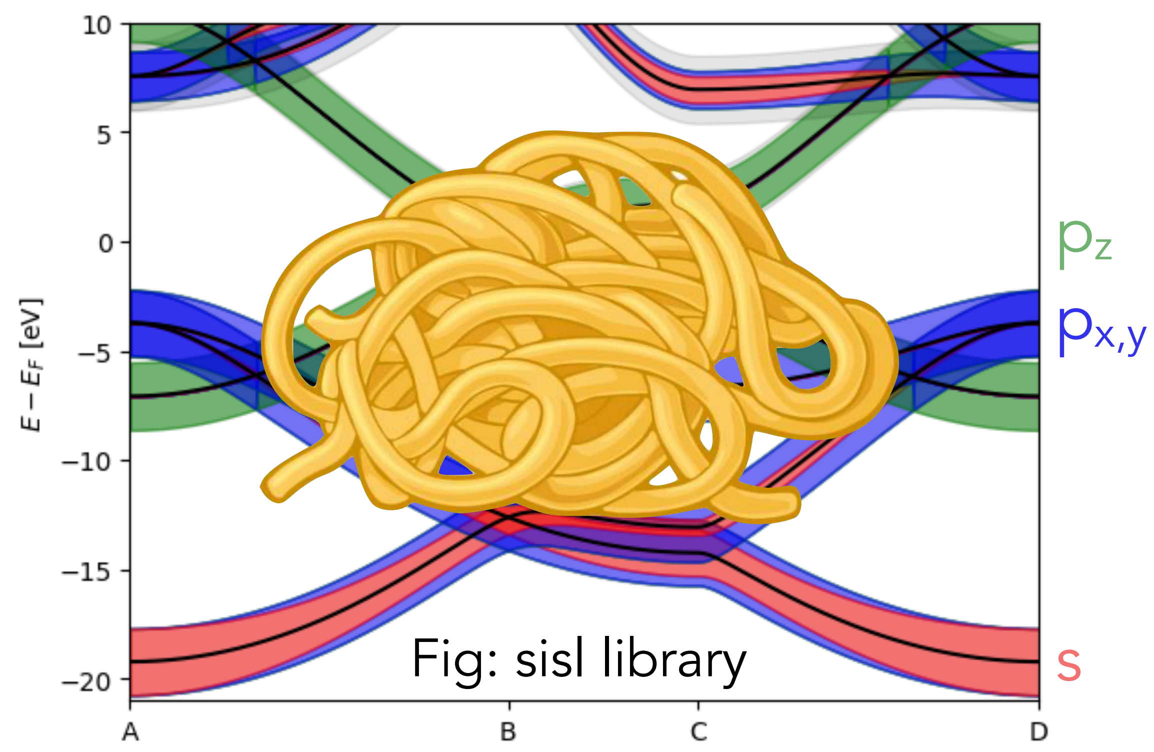
The energy levels form an "energy band" in the limit of many atoms, e.g., N ~ 10^{23}

Band structure of a crystal has many bands corresponding to different orbitals

Example:

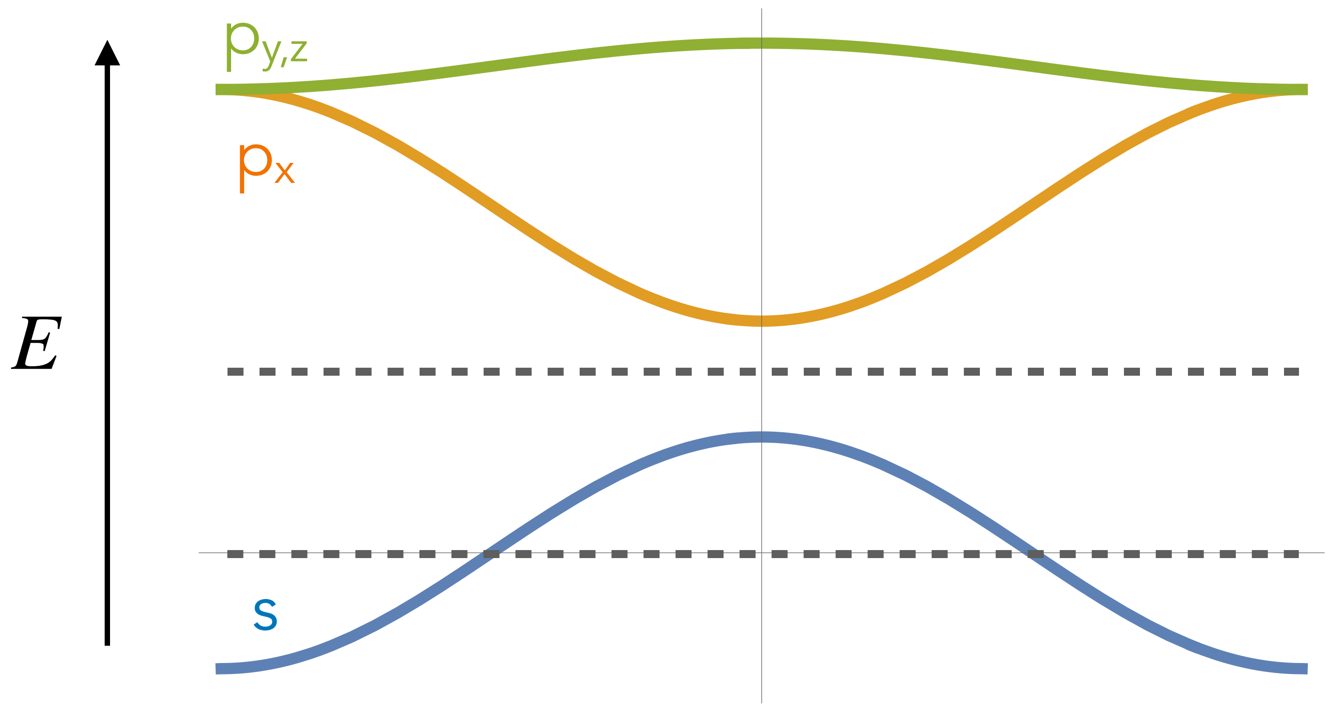


More realistic: graphene



How to distinguish metal vs insulator?

Example:



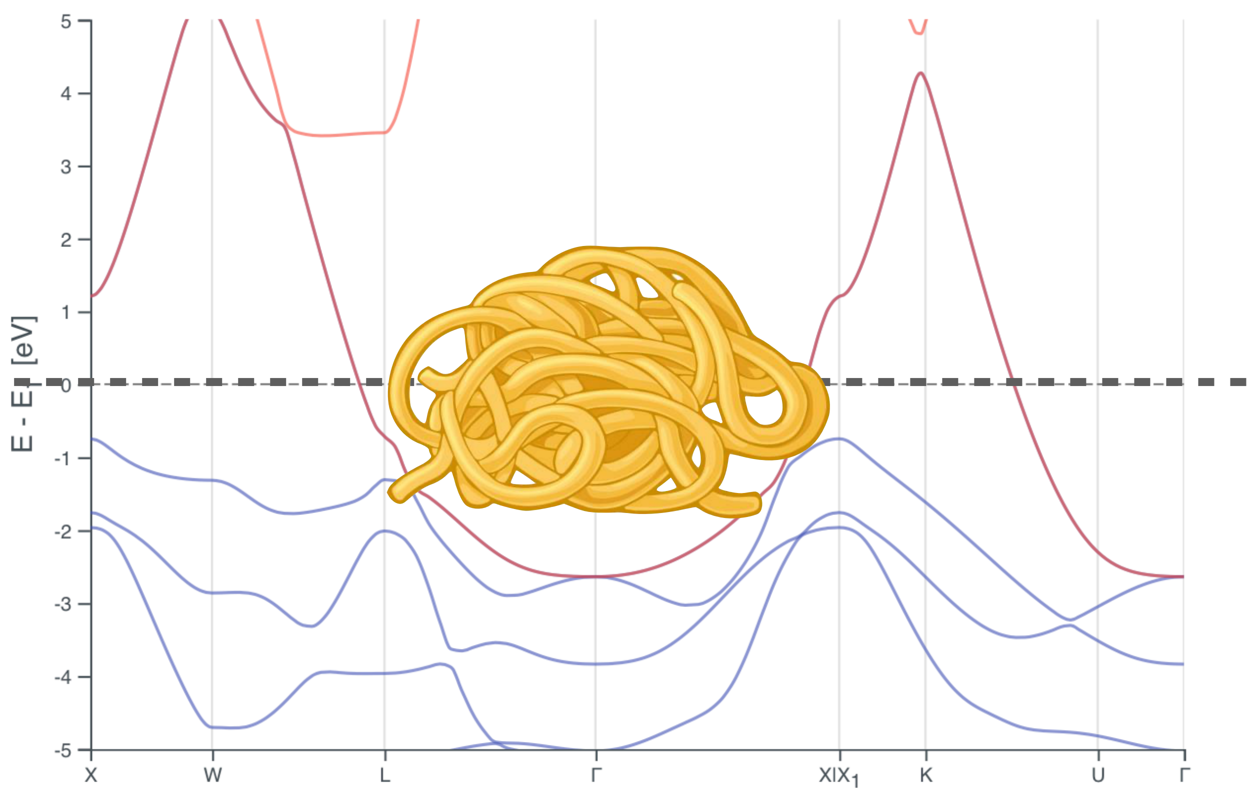
If 2 electrons per atom
⇒ band full ⇒ insulator

If 1 electron per atom
⇒ band half full ⇒ metal

Partially filled band = metal
Filled band = insulator

Real band structures: example of metal vs insulator

Band structure of gold (metal)



Band structure of diamond (insulator)

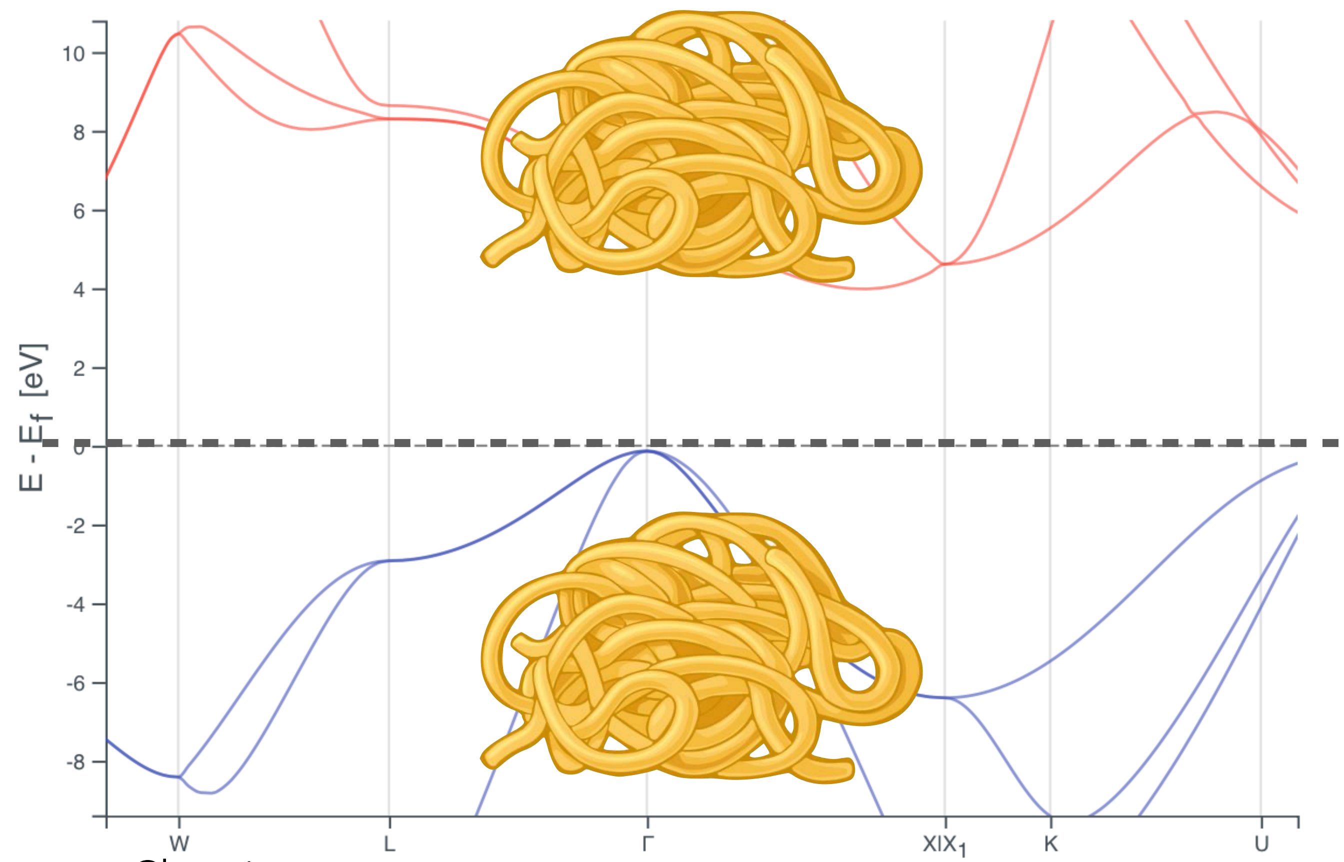


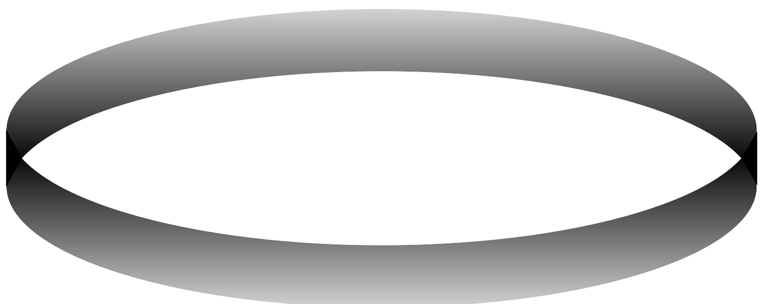
Fig: TopologicalQuantumChemistry.com

Partially filled band = metal

Filled band = insulator

What is topology?

Topologically equivalent manifolds can be smoothly deformed into each other



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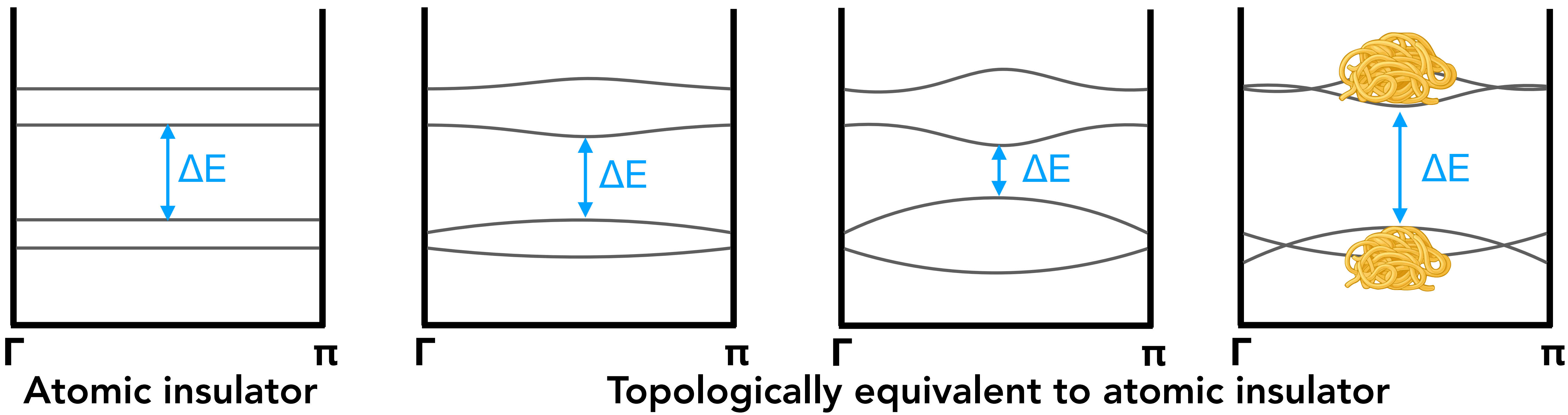
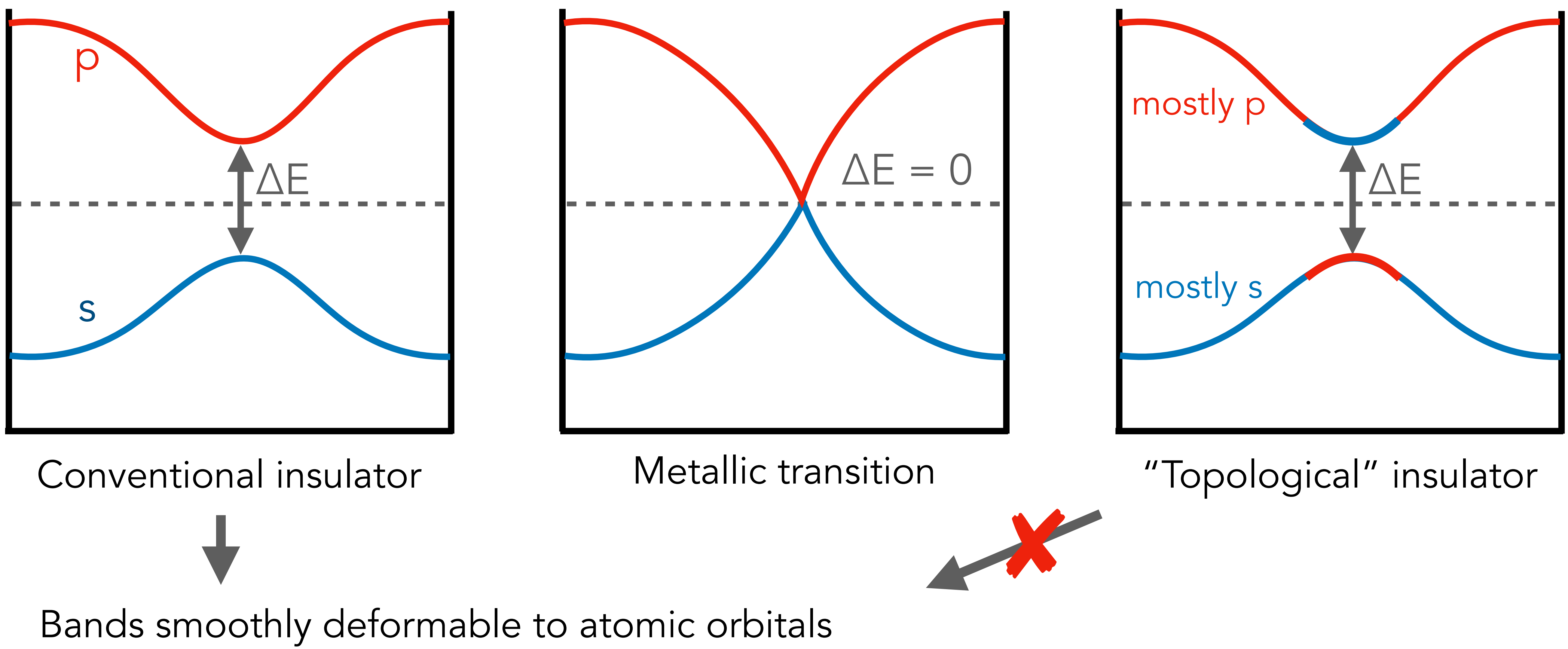
How does topology apply to band structures?

Topologically equivalent band structures can be smoothly deformed without closing an energy gap



"Equivalence classes" of insulators:
smoothly deform bands, and stay an insulator

Conventional: each energy band associated with an orbital

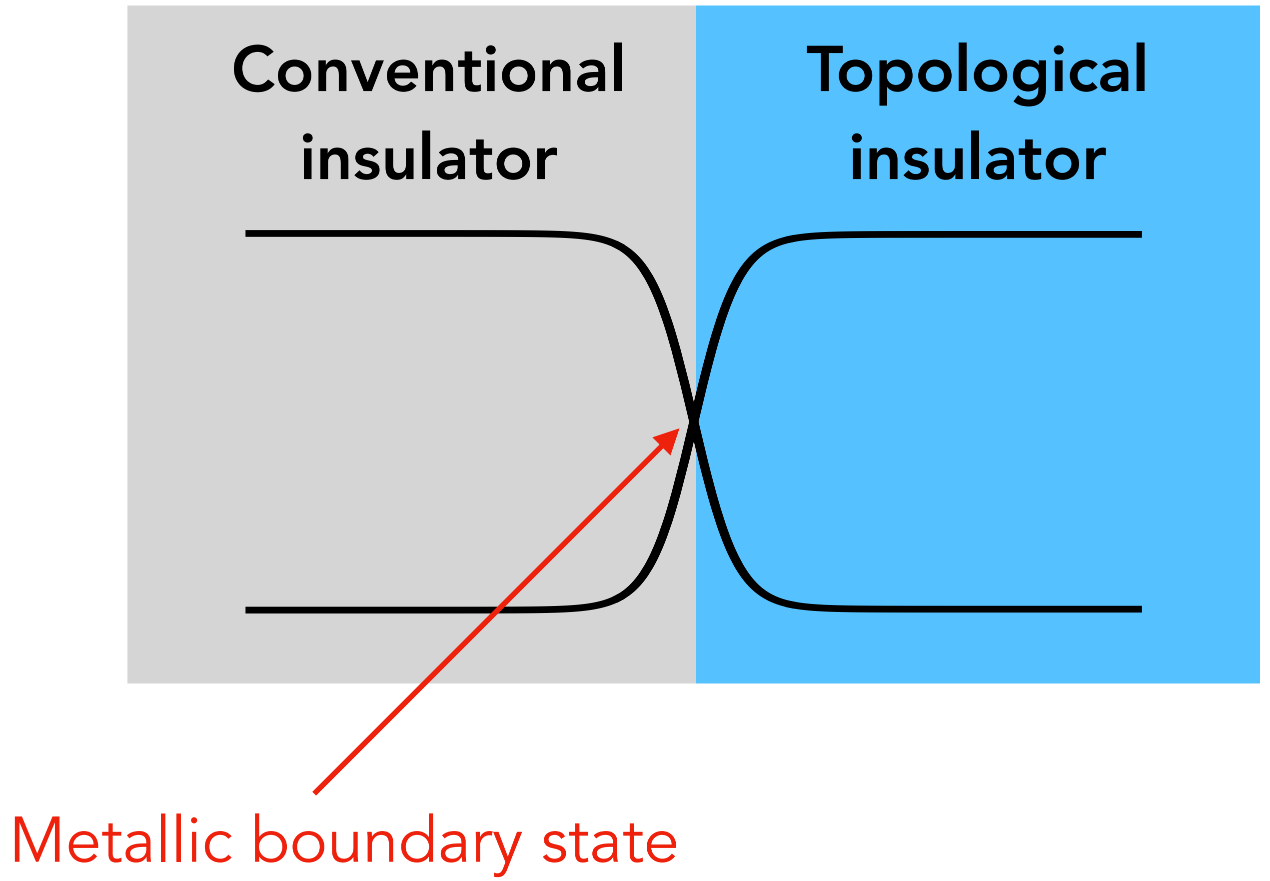


Topological insulators: bands cannot be associated with a single orbital

Why do topological insulators have metallic surfaces?

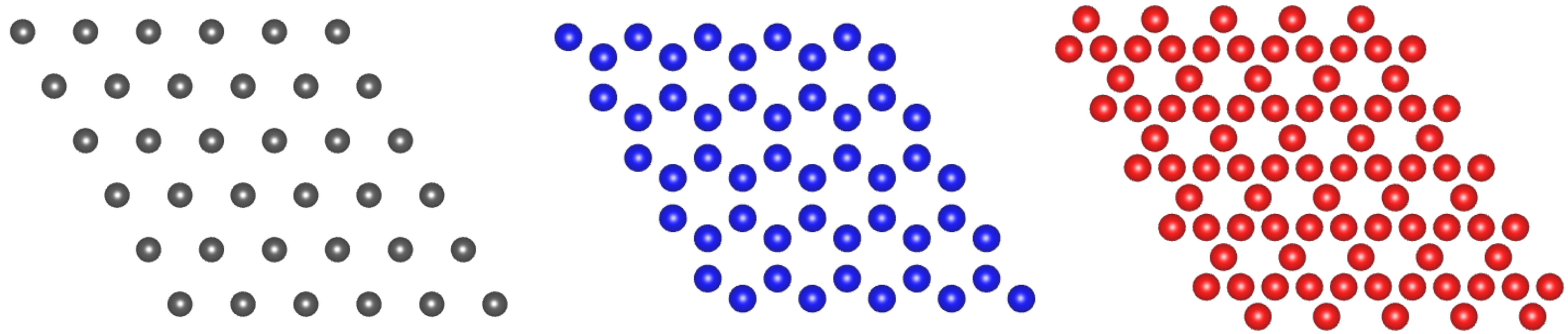
Cannot smoothly deform without closing the energy gap

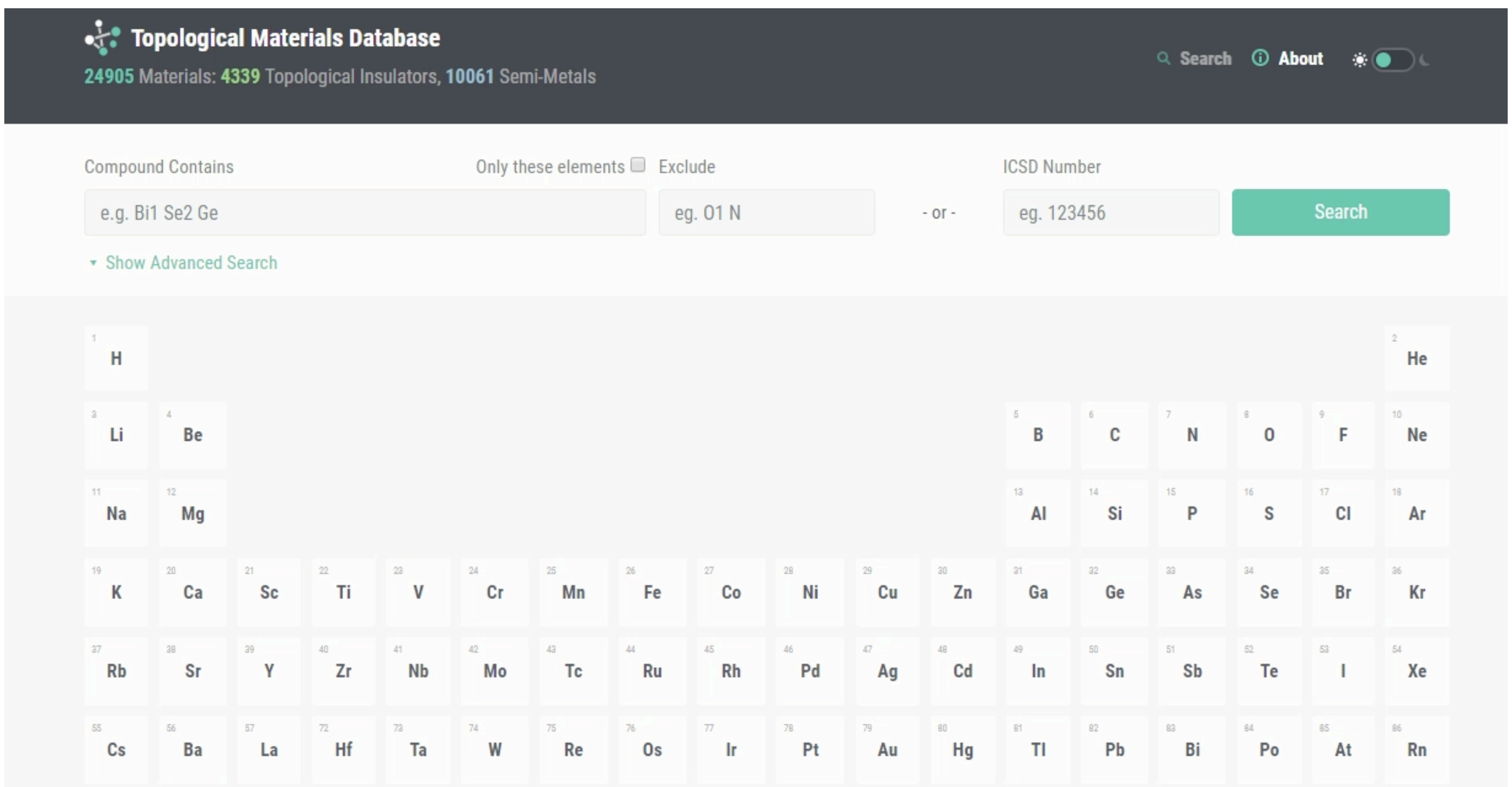
⇒ interface is metallic!



A little flavor of recent research topics

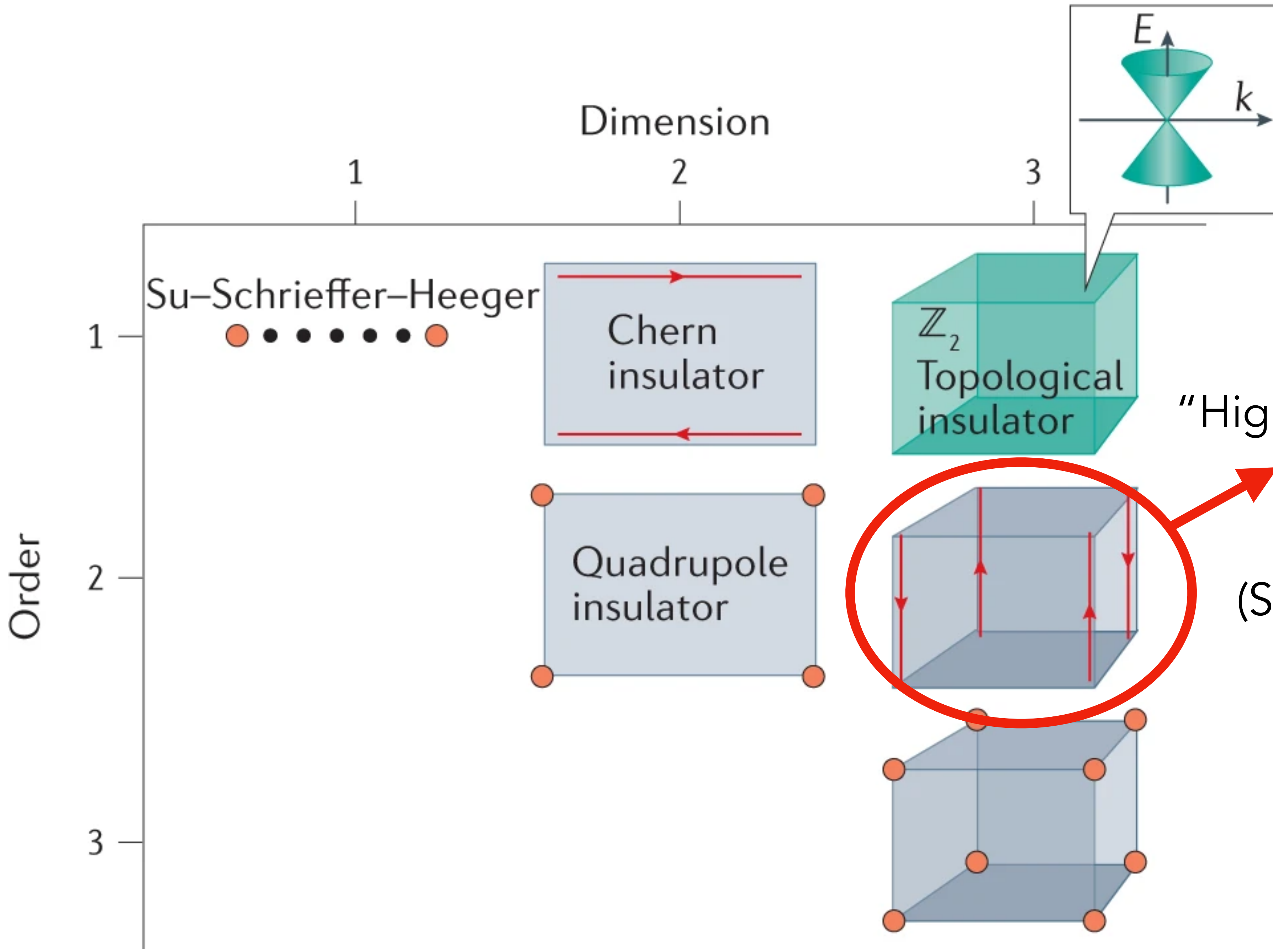
How does crystal symmetry impact topological phase?





TopologicalQuantumChemistry.com

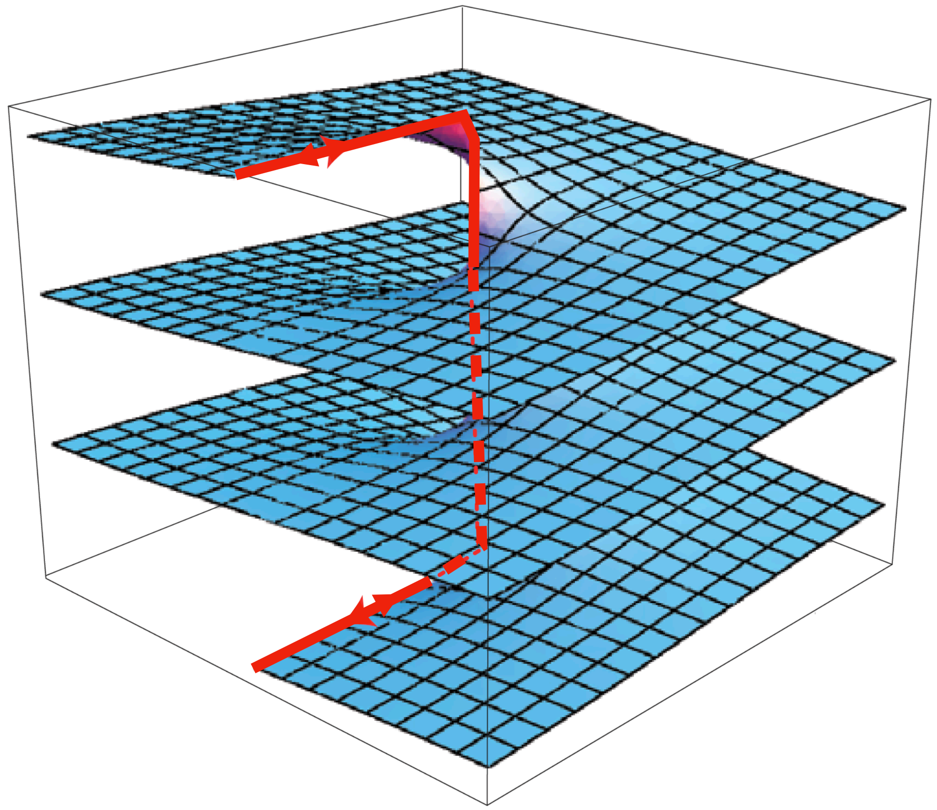
Refined classification of topological phases

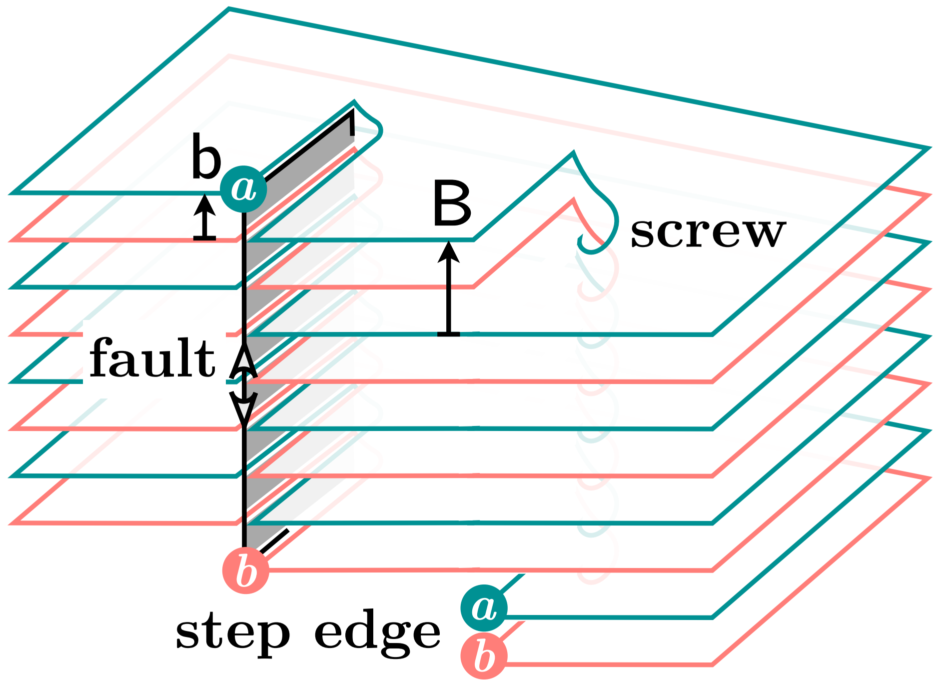


"Higher order topological insulator"
Metallic corner states!
Predicted in Bismuth
(Schindler et al Sci. Adv. 2018)

Fig: *Nature Reviews Materials* (2021)

Crystal defects as a probe of topology





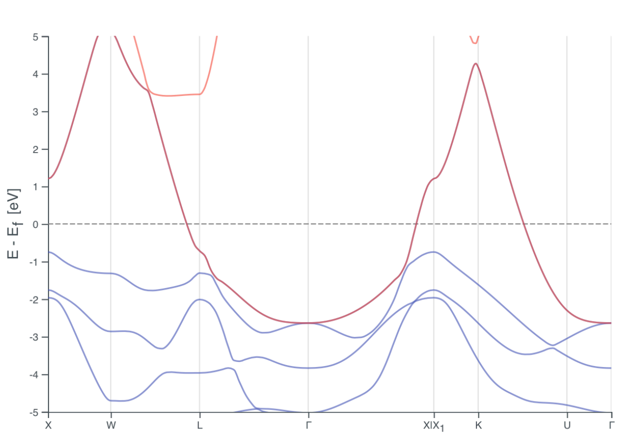
Figs: *Nature Phys* (2009), *Phys Rev Lett* (2019)

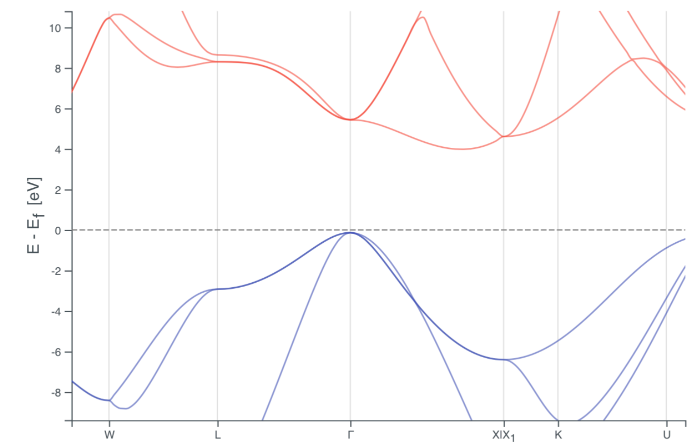
Summary

Electron energy levels in a crystal form energy bands

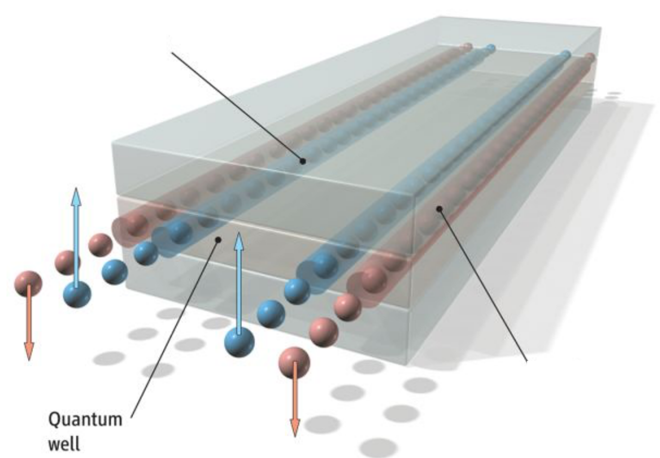
Partially filled bands ⇒ metal

Completely filled bands ⇒ insulator

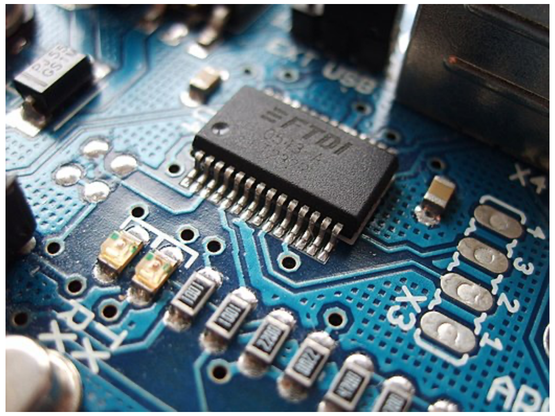




Topologically equivalent manifolds can be smoothly deformed into each other



Topology refines our classification of insulators



Not just a mathematical abstraction!
Metallic surface states useful to carry current efficiently; control electron spin; create topological qubits; and … ???