MAX PLANCK INSTITUTE
FOR CHEMICAL PHYSICS OF SOLIDS

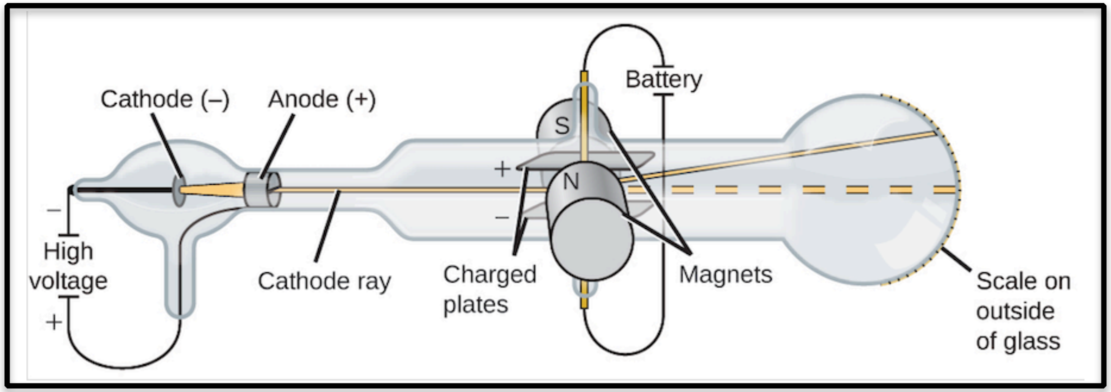
Topological Quantum Chemistry: The Topological Materials Database

QuMat October 2022

Maia G. Vergniory

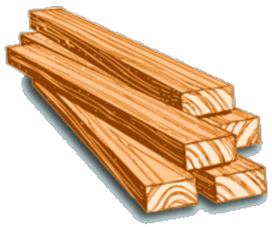
Introduction

Topological materials: second revolution in quantum mechanics



Classification as a function of conductivity

Insulators



Semiconductors

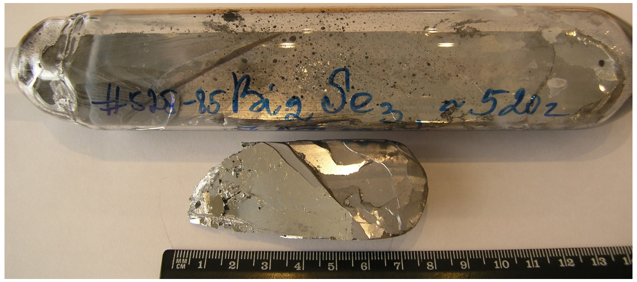
Metals

Introduction

What's a topological insulator?

New classification of matter

Topological Insulator



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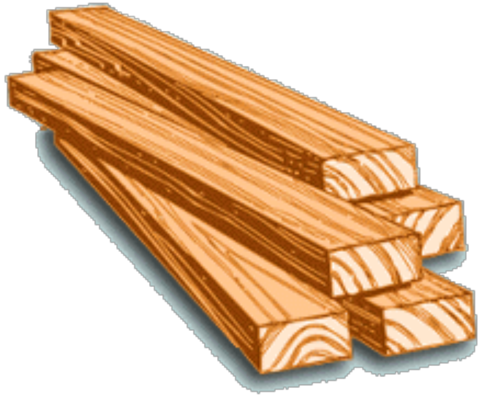


+

Insulator

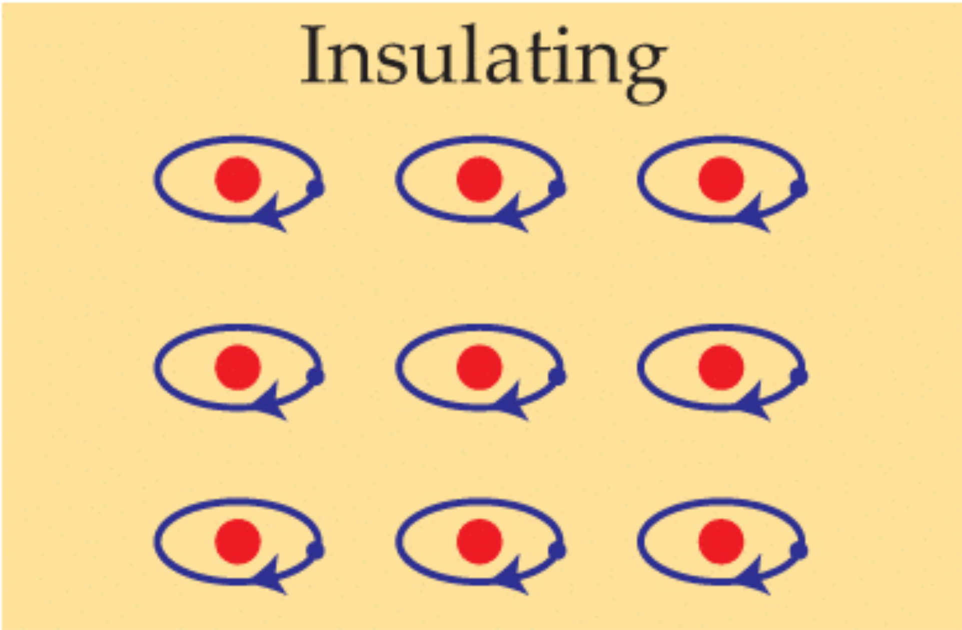
Metal

[Klitzing '80, Laughlin '83]

[Haldane '83]

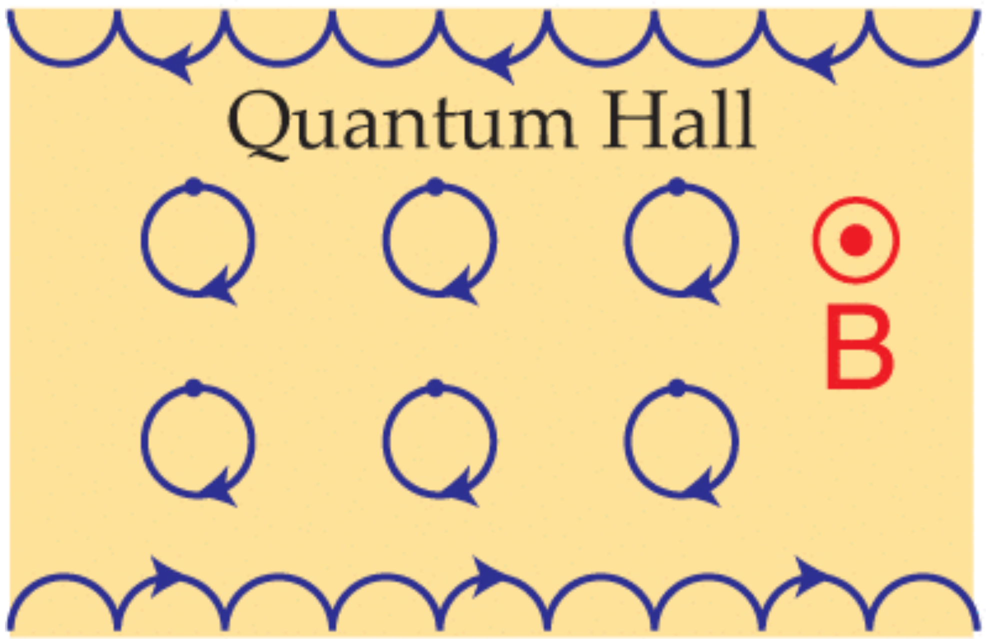
Introduction

Non-topological (trivial) insulator



Introduction

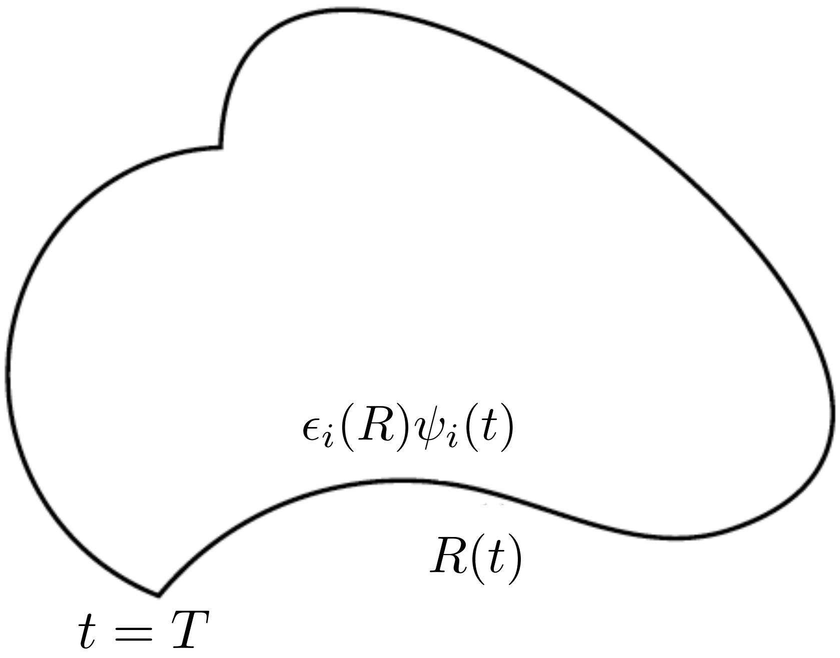
Quantum Hall Effect : bulk-boundary correspondence



K. v. Klitzinget al. Phys. Rev. Lett. 45, 494 (1980)

Introduction

Berry phase



Geometrical phase

$$\psi_i(t) = e^{-i\int \epsilon_i R(t)dt} e^{-i\chi(t)} \phi(R(t))$$

$$t = T$$

$$\chi(T) \neq 0$$

Chern number

$$\sigma_h = n\frac{e^2}{h}$$

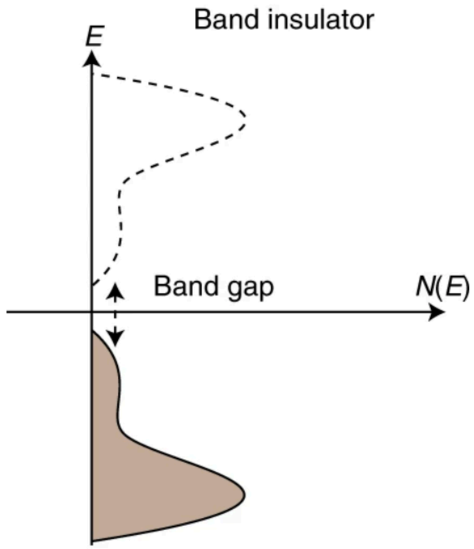
Hall conductivity

M. Berry 1984

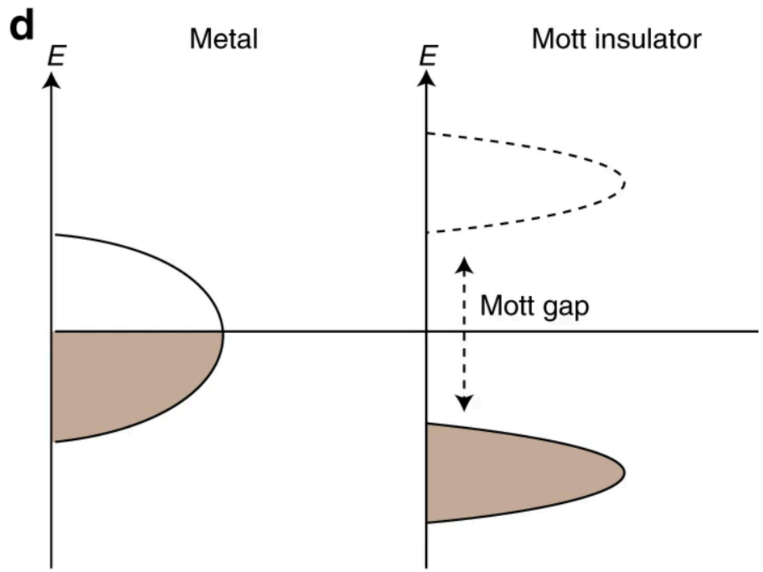
Introduction

Insulators

Band insulators



Correlated insulators



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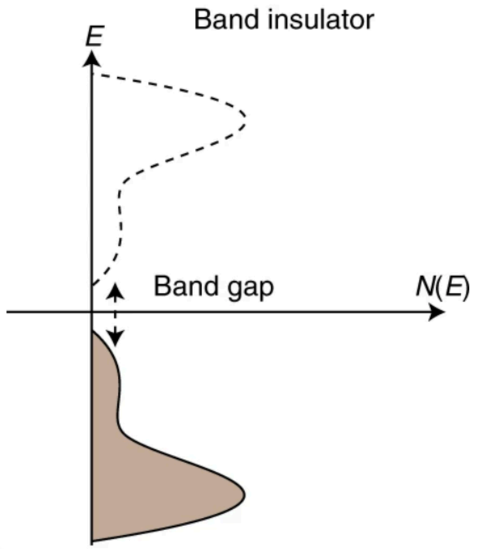
Insulators

Band insulators



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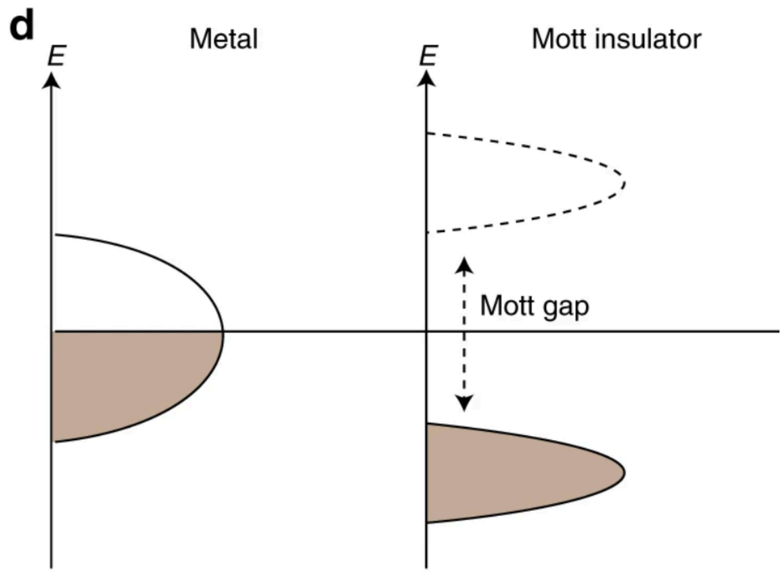
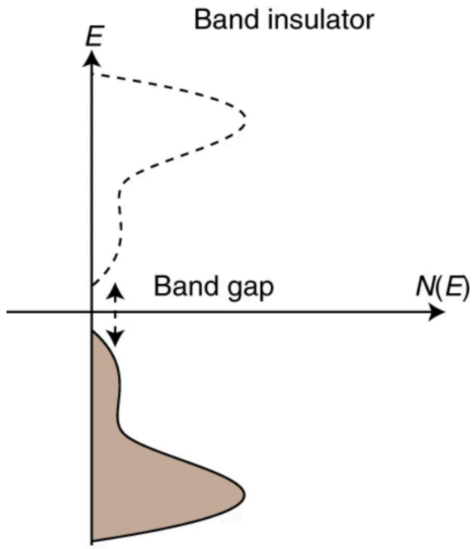


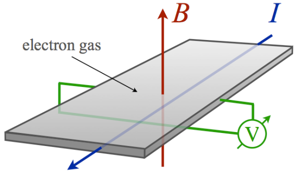
Insulators

Band insulators



Topology and symmetry

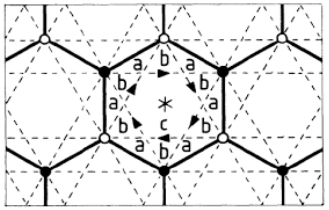
Quantum Hall effect (edge states)



1980

Time-Reversal Symmetry broken
External **B** (2D), low Tº

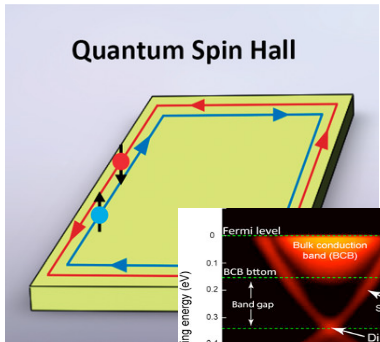
Chern insulators (edge states)

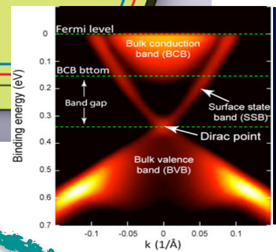


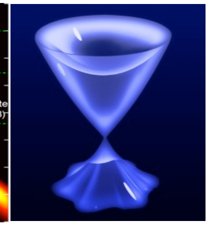
1988

Time-Reversal Symmetry broken
Intrinsic magnetism (2D)

Quantum spin Hall effect



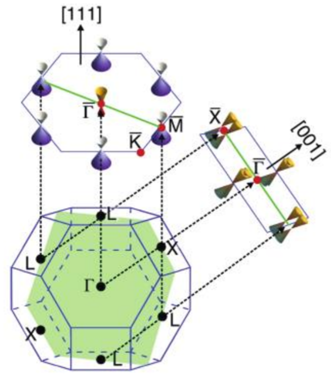




3D TIs

2005

Time-Reversal preserved
Strong SOC, 2D and 3D



3D TCIs

2011

Mirror symmetry

K. v. Klitzinget 1980, Haldane 1988, Kane and Mele 2005, Liang Fu 2011

Topological classification before crystalline symmetries

$\Theta H(\mathbf{k})\Theta^{-1} = +H(-\mathbf{k})$; $\Theta^2 = \pm 1$ ⟶ Time Reversal

$\Xi H(\mathbf{k})\Xi^{-1} = -H(-\mathbf{k})$; $\Xi^2 = \pm 1$ ⟶ Particle - Hole

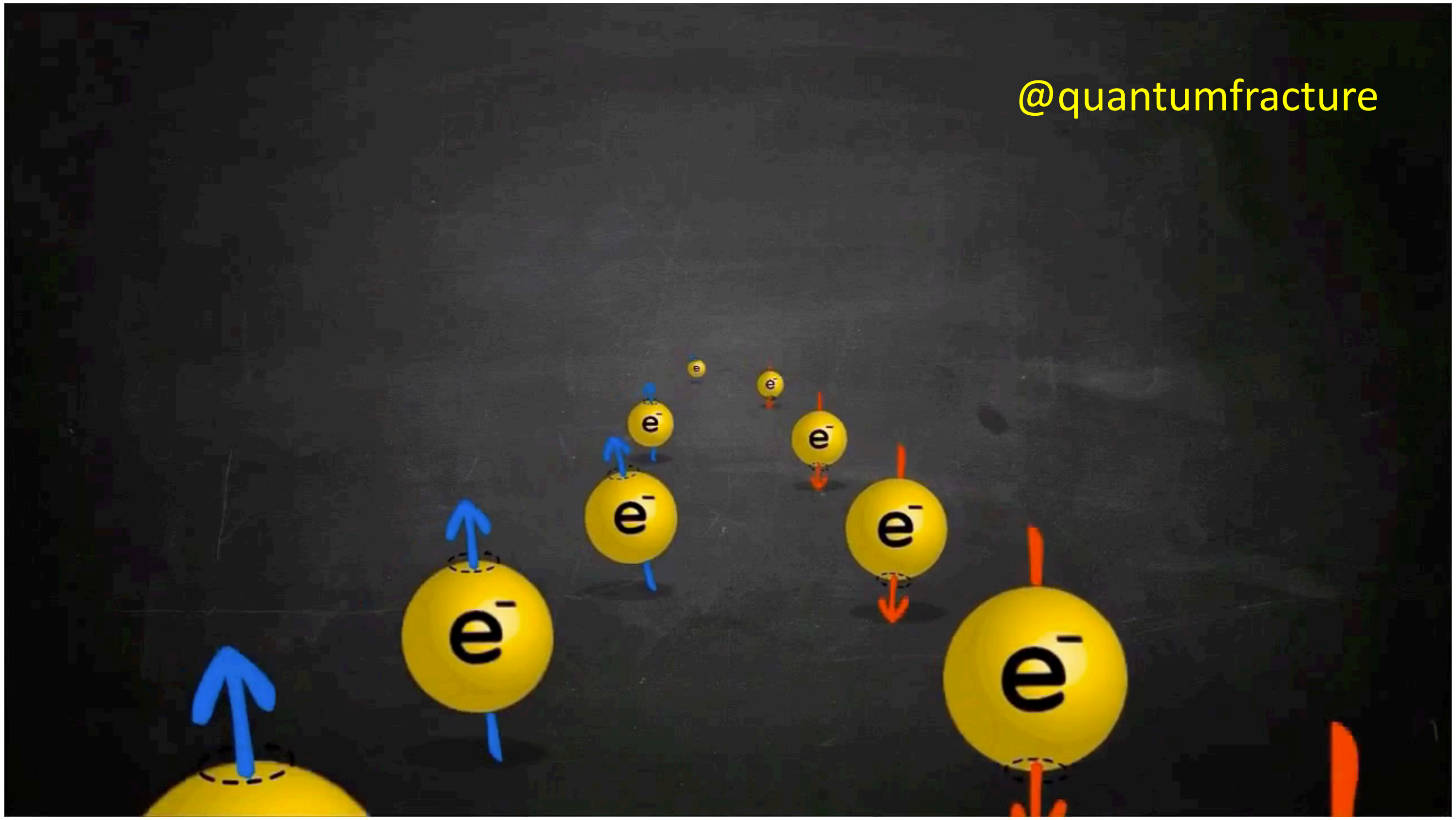
$\Pi H(\mathbf{k})\Pi^{-1} = -H(\mathbf{k})$; $\Pi \propto \Theta\Xi$ ⟶ Chiral symmetry

Altland-Zirnbauer Random Matrix Classes

Symmetry				d							
AZ	Θ	Ξ	Π	1	2	3	4	5	6	7	8
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
DIII	-1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0
AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
C	0	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	1	-1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

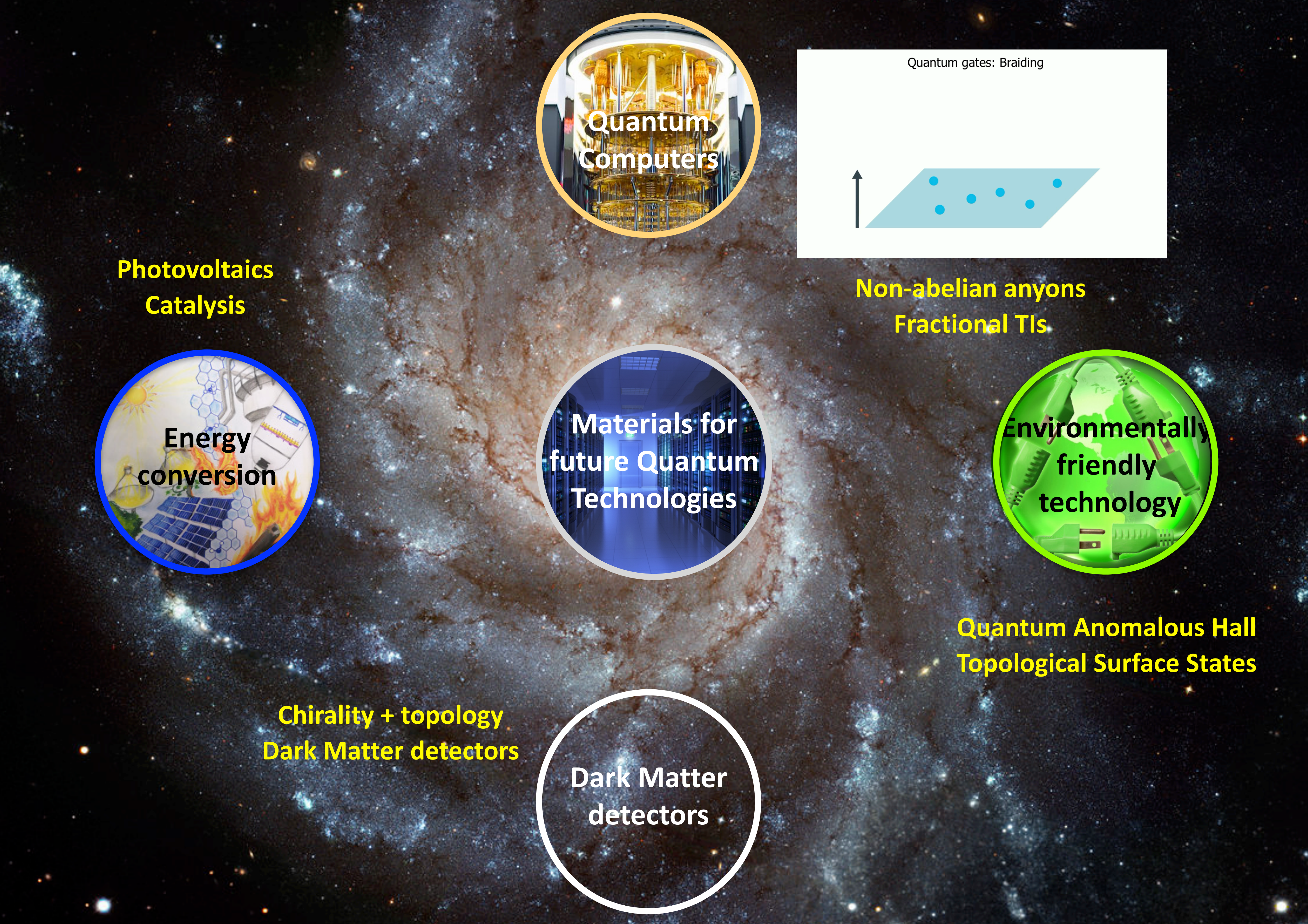
Ryu, Schnyder, Furusaki, Ludwig New J. Phys. 12, 065010 (2010)

Introduction



Unstoppable currents, constant conductivity, spin-momentum locking (in 2D and 3D)
Independent of size, weak disorder and temperature

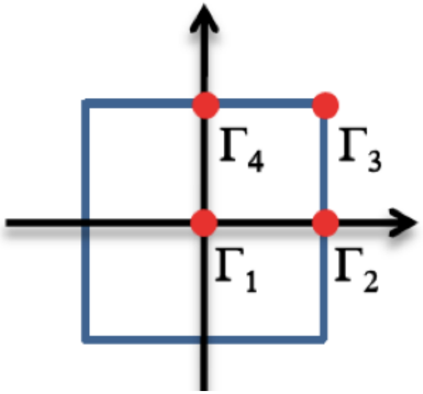
C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005)

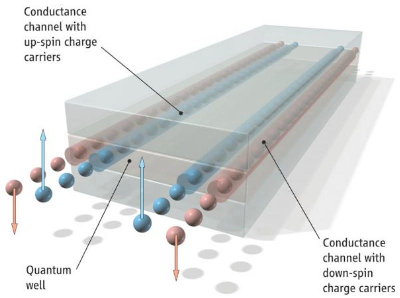


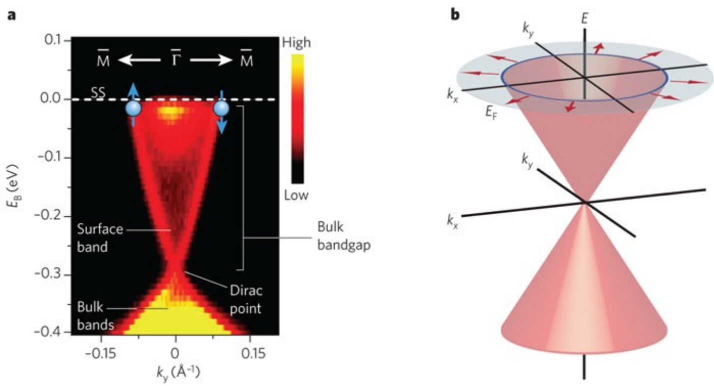
Quantum Computers
Quantum gates: Braiding
Photovoltaics
Catalysis
Non-abelian anyons
Fractional TIs
Energy conversion
Materials for future Quantum Technologies
Environmentally friendly technology
Quantum Anomalous Hall
Topological Surface States
Chirality + topology
Dark Matter detectors
Dark Matter detectors

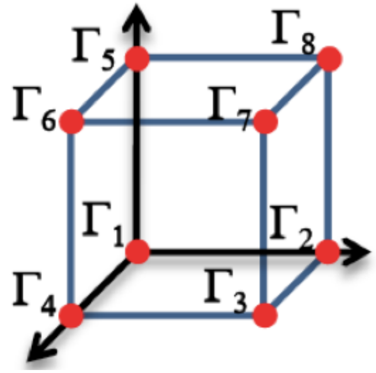
Topological classification before crystalline symmetries

Example: Z_2 invariant in 2D and 3D Topological Insulators (protected by TRS)
Band theory (Fu, Kane & Male (2007), Moore and Balents (2007), Roy (2007)







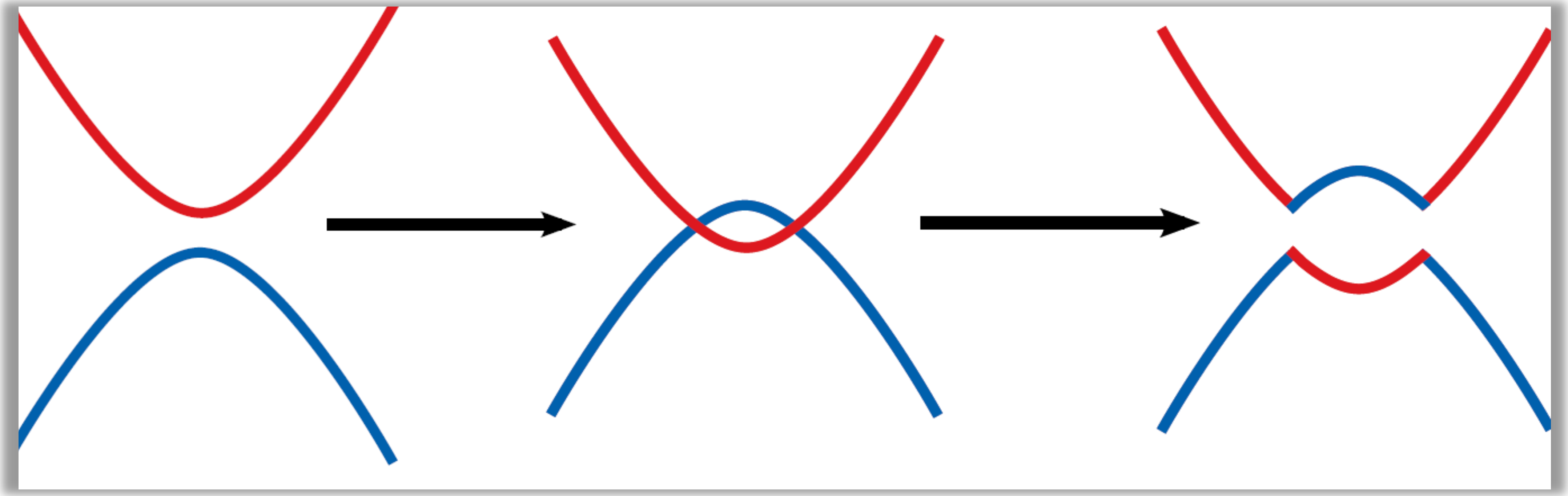


$$W_{nm}(k_x, k_y) = \overline{\exp}\left[\int_0^{2\pi} \mathrm{d}k_z \langle u_m(\vec{k})|\partial_{k_z}|u_n(\vec{k})\rangle\right]$$

unitary operator in filled band subspace

occupied band eigenstates

Band inversion criteria



$$(-1)^{\nu} = \Pi\delta i = \pm 1$$

$\nu =$ { -1 topological insulator
1 trivial insulator

Band inversion criteria

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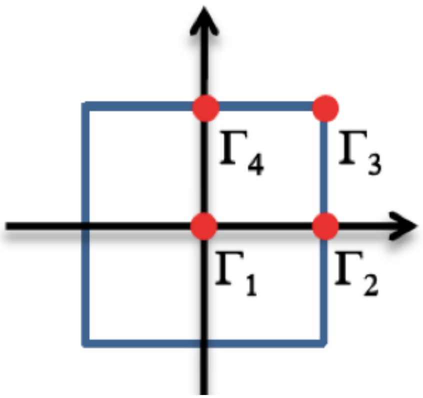

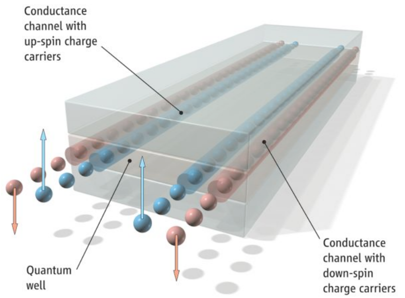

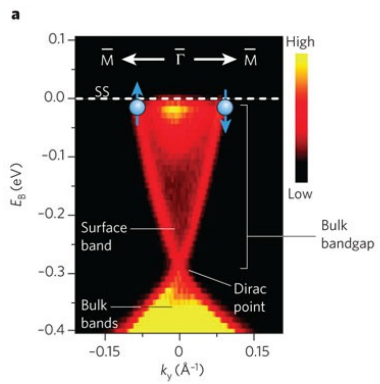

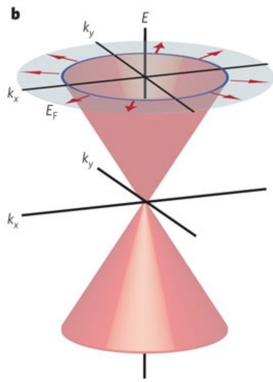

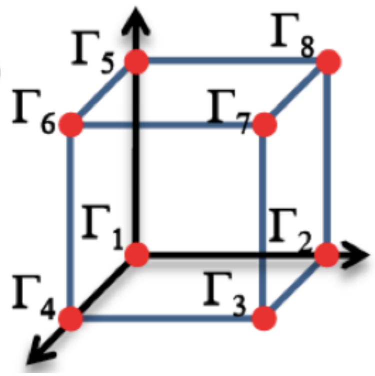

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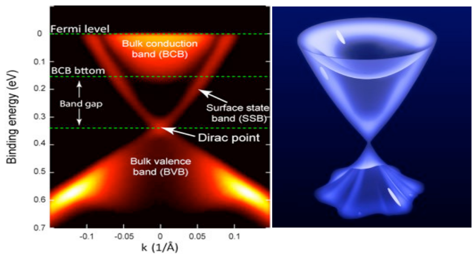
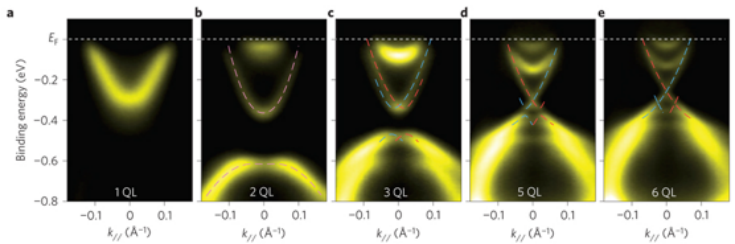
Topological materials



Hsieh Nature (2008)
Zhang Nat Phys (2009)
Xia Nat Phys (2008)

3D TIs theory + exp protected by TRS : Bi_2Se_3



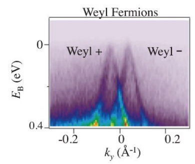
Chang Science (2013)

QAHE

Weng PRX (2015)
Xu Science (2015)

Weyl semimetals

Discovery of a Weyl fermion semimetal and topological Fermi arcs



Bradlyn (2016)

New Fermions

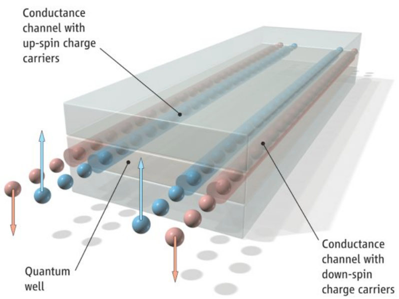
Nodal Lines

Bzdušek (2016)

2006	2007	2008	**2009**	2010	**2011**	2012	2013	**2014**	2015	2016	2017	2018

Prediction HgTe 2D TI

Bernevig Science (2006)
König Science (2007)



Kane & Mele, PRL (2015)

Hsieh Nat Comm (2012)
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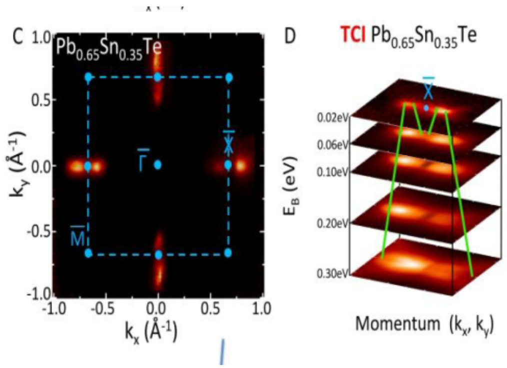


Mirror Chern insulators

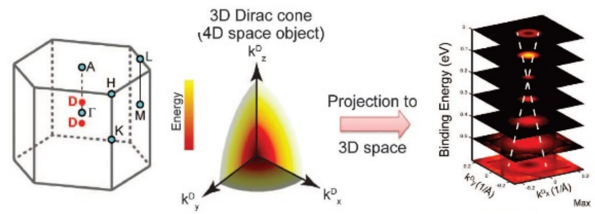
Type II Weyls

Soluyanov (2015)

Dirac semimetals

Discovery of a Three-Dimensional Topological Dirac Semimetal, Na_3Bi

Z. K. Liu,[1*] B. Zhou,[2,3*] Y. Zhang,[3] Z. J. Wang,[4] H. M. Weng,[4,5] D. Prabhakaran,[2] S.-K. Mo,[3] Z. X. Shen,[1] Z. Fang,[4,5] X. Dai,[4,5] Z. Hussain,[3] Y. L. Chen[2,6]†

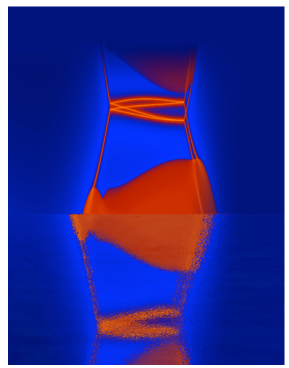


High Order TIs

Schindler (2018)

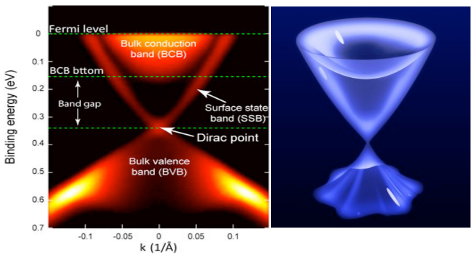
Non-symmorphic TIs

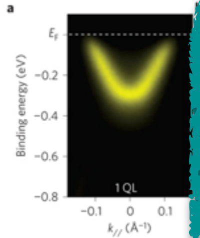
Alexandrinata (2016)

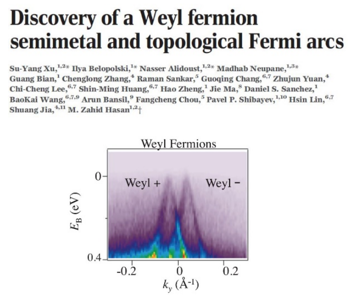


Topological materials

Crystalline symmetries



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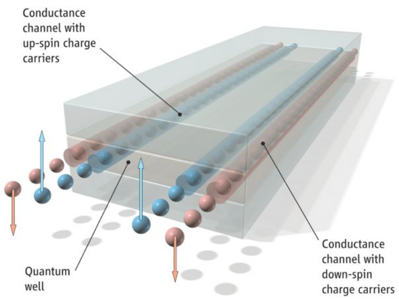

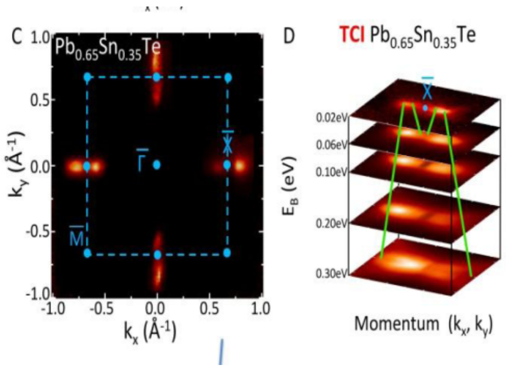

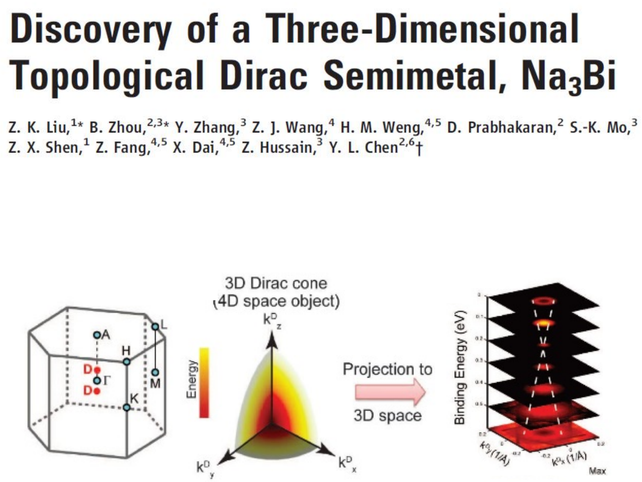
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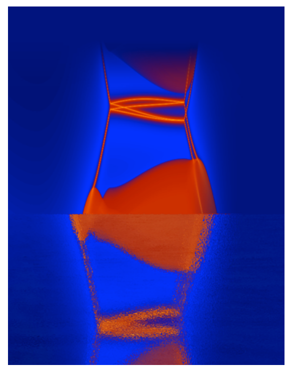
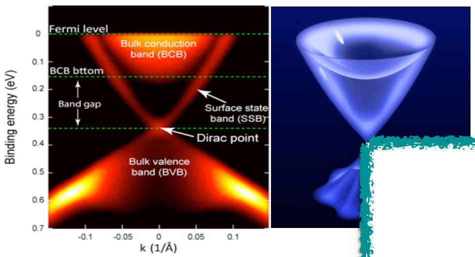


Kane & Mele, PRL (2015)

Topological materials



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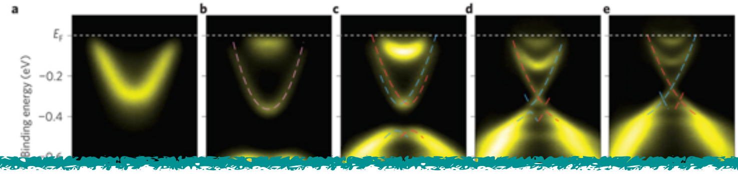
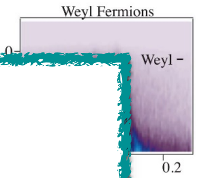


Discovery of a Weyl fermion semimetal and topological Fermi ar...

Su-Yang Xu, Ilya Belopolski, Nasser Alidoust, Madhab Neupane, Guang Bian, Chenglong Zhang, Raman Sankar, Guoqing Chang, Zhujun Yuan, Chi-Cheng Lee, Shin-Ming Huang, Hao Zheng, Jie Ma, Daniel S. Sanchez, BaoKai Wang, Arun Bansil, Fangcheng Chou, Pavel P. Shibayev, Hsin Lin, Shuang Jia, M. Zahid Hasan



...adlyn (2016)

Nodal Lines

Bzdušek (2016)

2006	2007	20...	...16	2017	2018

2018 (40 years)

~300 topological materials

High Order TIs

Schindler (2018)

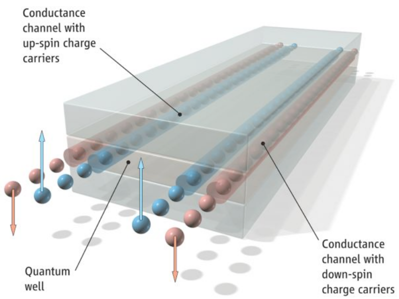
Prediction
HgTe 2D TI

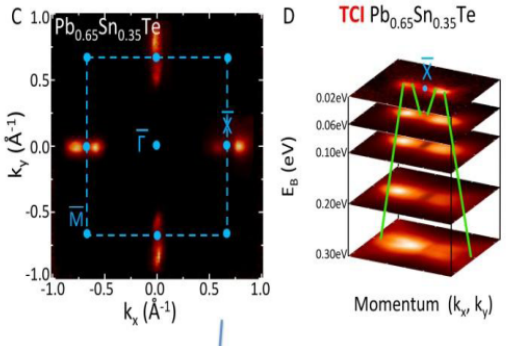
Bernevig Scien...
König Science (...

...symmorphic TIs

Alexandrinata (2016)

Tanaka Nat Phys (2012)





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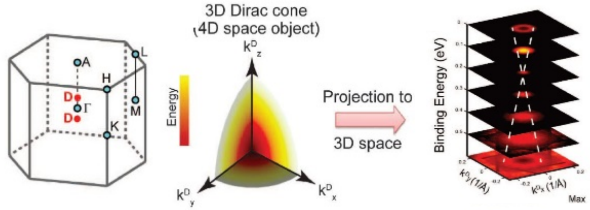
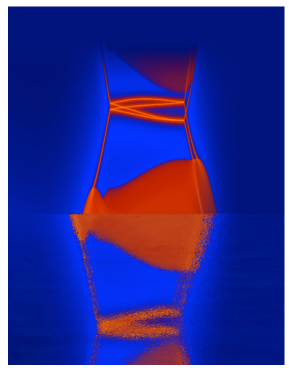




Kane & Mele, PRL (2015)

Crystal Structure

230
Space-Groups

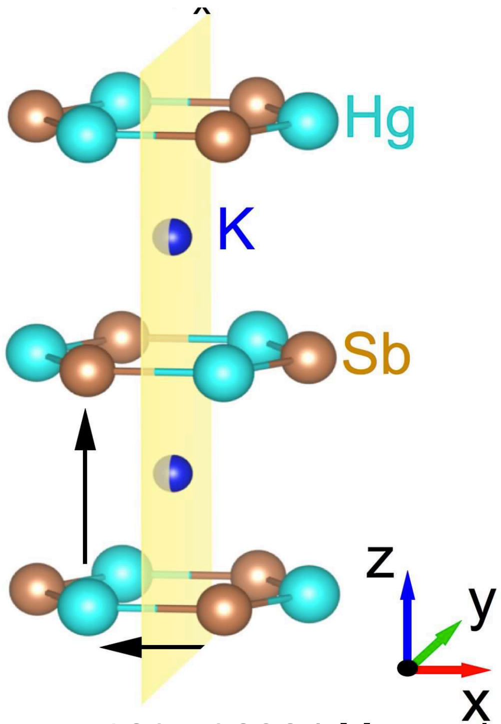
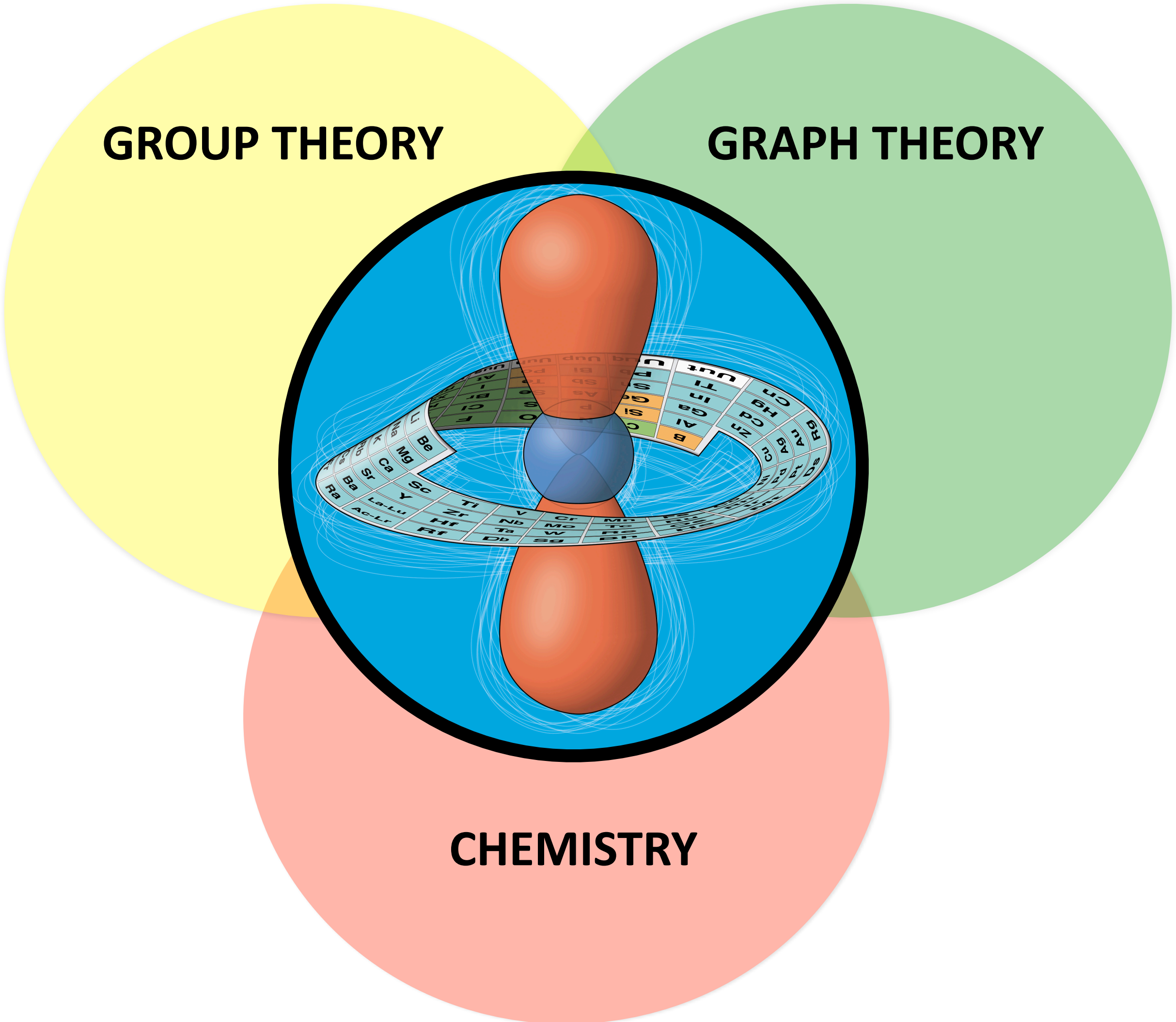


Image: 1605.06824 Ma et al

Ingredients:

- unit lattice translations ($\mathbf{Z}^3$)
- point group operations (rotations, reflections)
- non-symmorphic (screw, glide)
- orbitals
- atoms in some lattice positions

Topological Quantum Chemistry

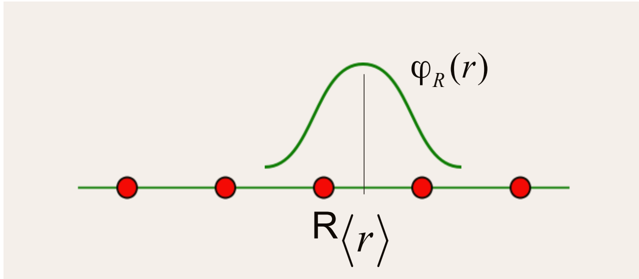


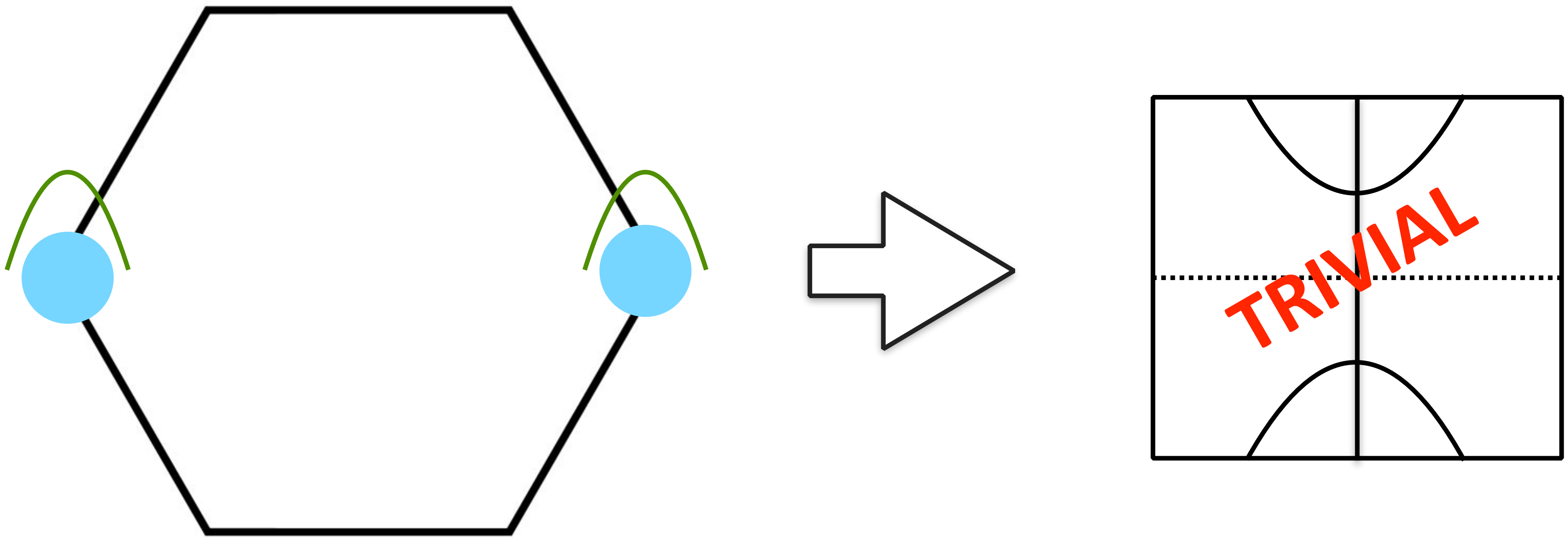
Nature (2017)

Atomic limit

Bloch states $\psi_k(r) = e^{ikr} u_k(r)$ are defined for periodic boundary conditions
Define localized **Wannier States** :

$$|\varphi(R)\rangle = \oint_{BZ} \frac{dk}{2\pi} e^{-ikR} |\psi_k\rangle = \oint_{BZ} \frac{dk}{2\pi} e^{-ik(R-r)} |u_k\rangle$$





Vanderbilt and Soluyanov PRB (2011)

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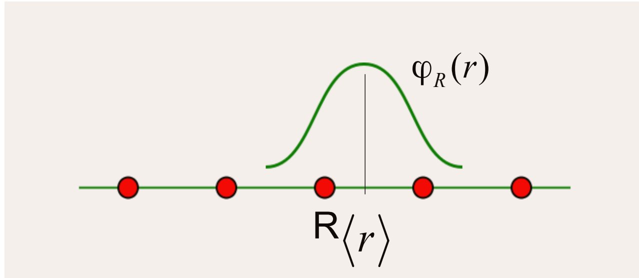
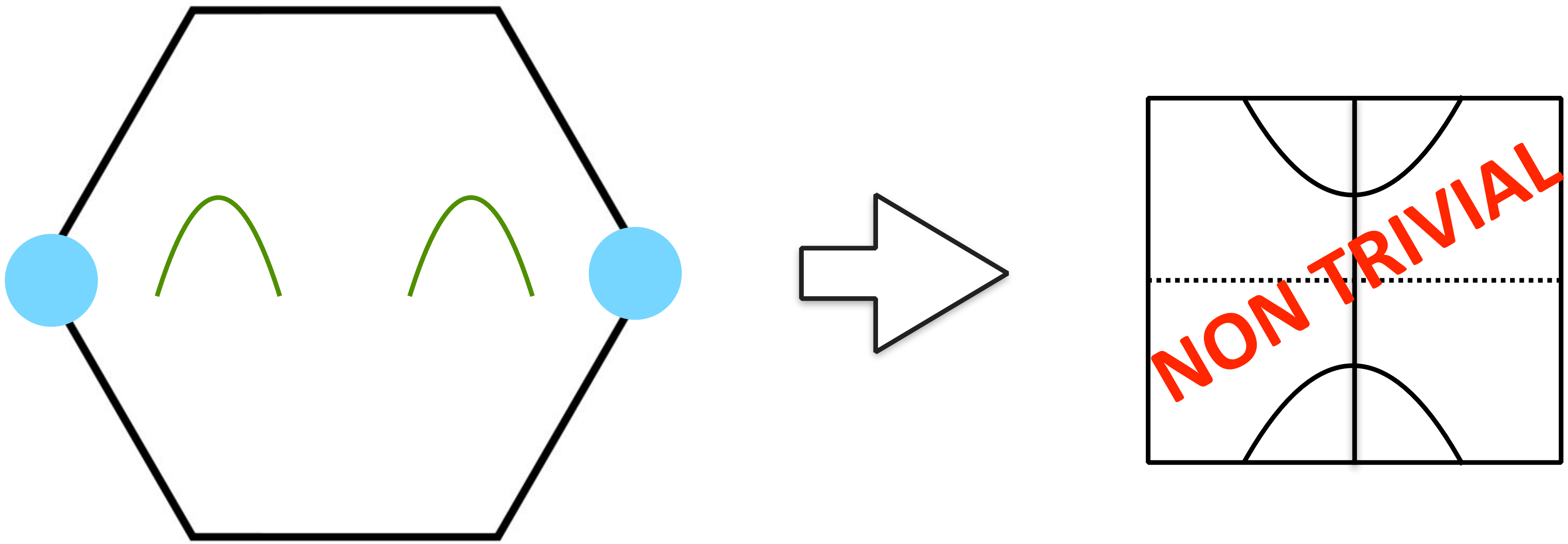




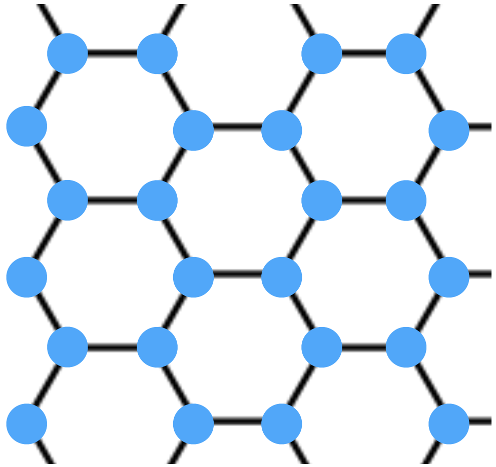
Vanderbilt and Soluyanov PRB (2011)

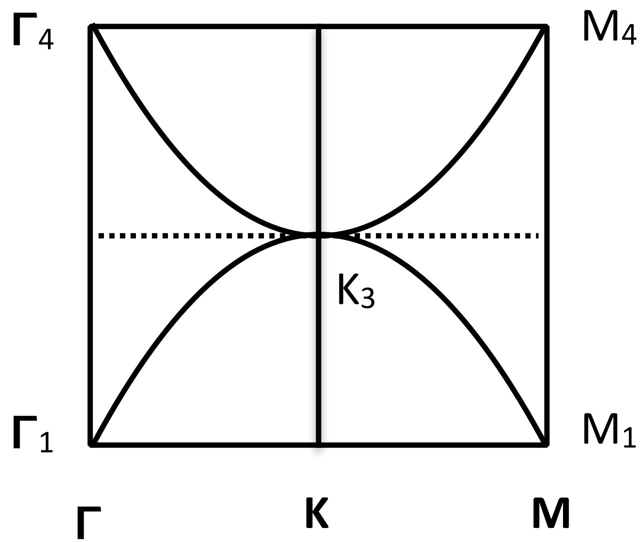
Elementary band representations (EBRs)

orbital + atomic site + lattice

(irrep + wyckoff position + space group)

s (or p_z) orbitals





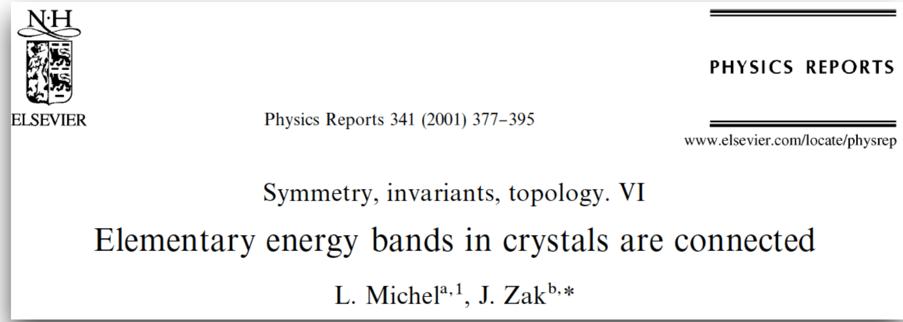
atomic limit = EBR

An EBR describes a set of Wannierizable bands

Zak, "Symmetry specification of bands in solids," Physical Review Letters 45, 1025 (1980), Band representations and symmetry types of bands in solids," Physical Review B 23, 2824 (1981), Band representations of space groups," Physical Review B 26, 3010 (1982).

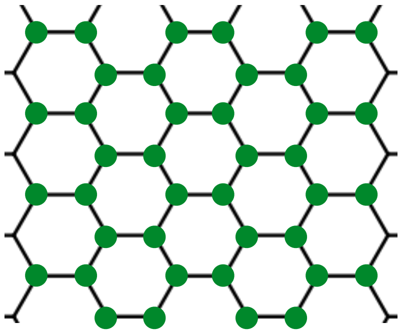
Elementary band representations (EBRs)

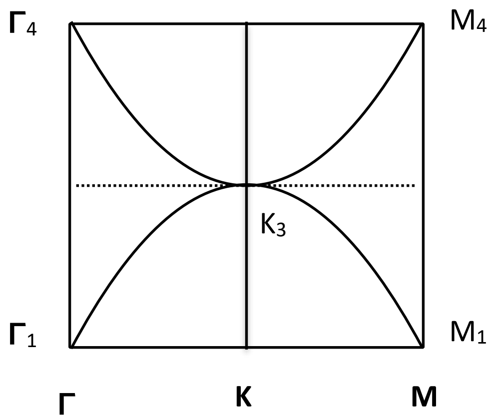
Elementary Band Representations


N H
ELSEVIER
Physics Reports 341 (2001) 377–395
PHYSICS REPORTS
www.elsevier.com/locate/physrep

Symmetry, invariants, topology. VI
Elementary energy bands in crystals are connected
L. Michel[a,1], J. Zak[b,*]

orbital + atomic site + lattice



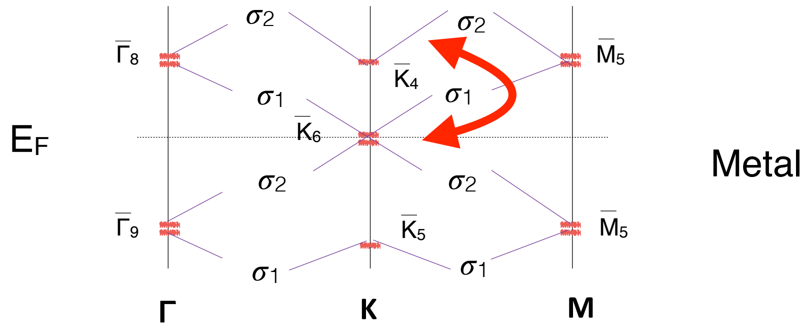


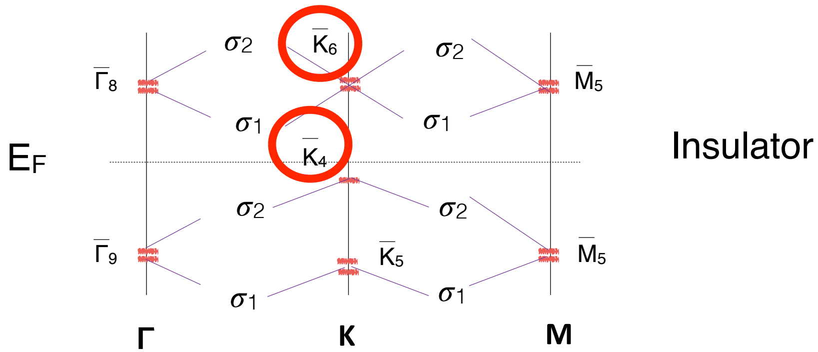
Compatibility Relations

All possible connection between maximal and non-maximal k-vectors

$\mathbf{k}_i\ (\mathbf{u}_1)=\mathbf{k}_1$
$\mathbf{k}_i\ (\mathbf{u}_2)=\mathbf{k}_2$

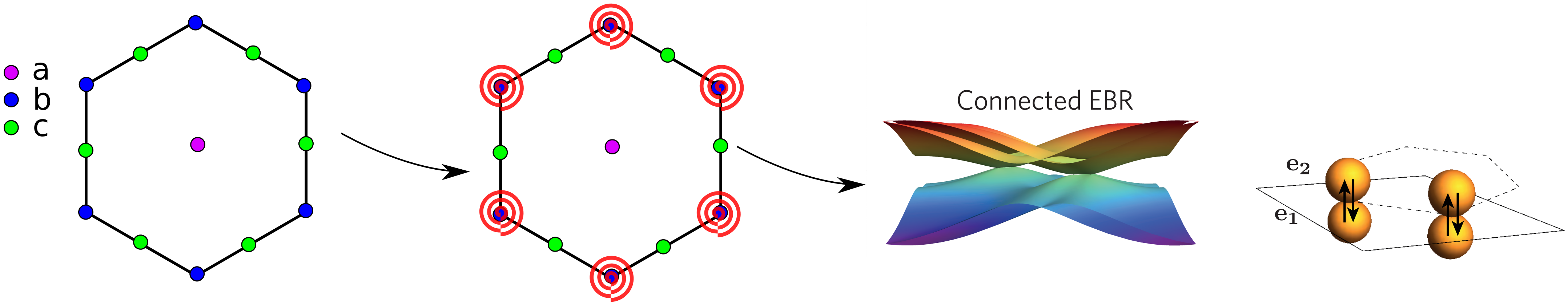
for each max. **k** in ***k** and $\mathbf{k}_i$ non-maximal





B. Bradlyn et al. Nature 547 (2017), M.G. Vergniory et al. Nature 566 (2019), M. G. Vergniory et al. Science (2022)

Topological Quantum Chemistry

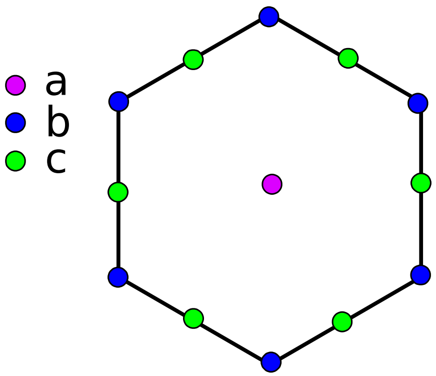


Maximal symmetry
Wyckoff positions

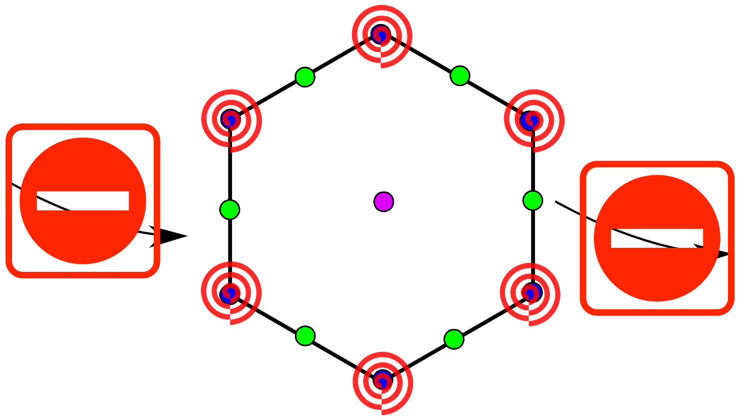
Wannier functions at
some Wyckoff pos.

Nature (2017)

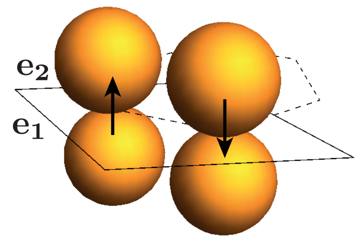
Topological Quantum Chemistry



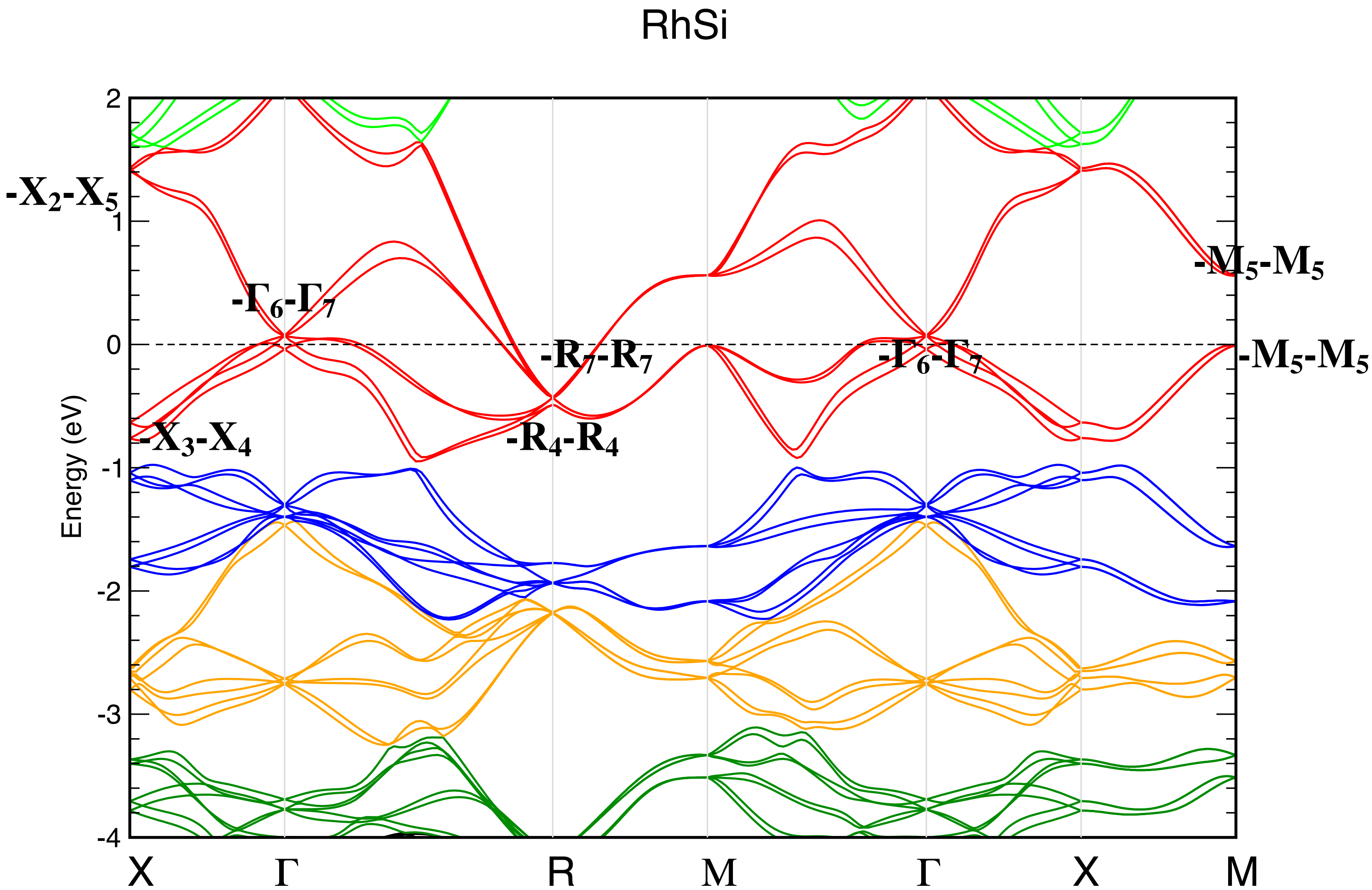
Maximal symmetry
Wyckoff positions



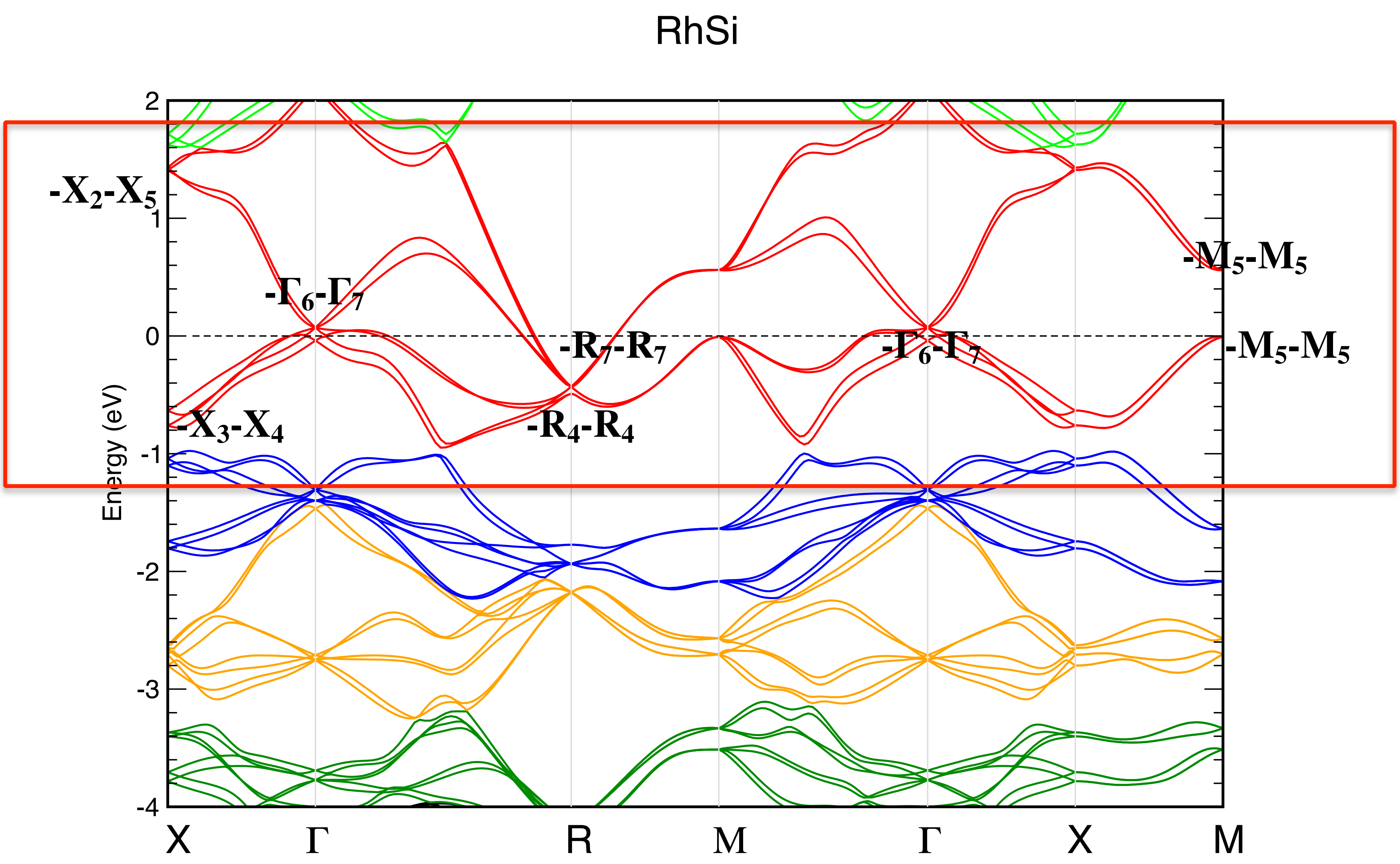
Wannier functions at
some Wyckoff pos.



Nature (2017)



RhSi
Energy (eV)
2
1
0
-1
-2
-3
-4
X
Γ
R
M
Γ
X
M
-X2-X5
-Γ6-Γ7
-X3-X4
-R7-R7
-R4-R4
-Γ6-Γ7
-M5-M5
-M5-M5


RhSi
Energy (eV)
2
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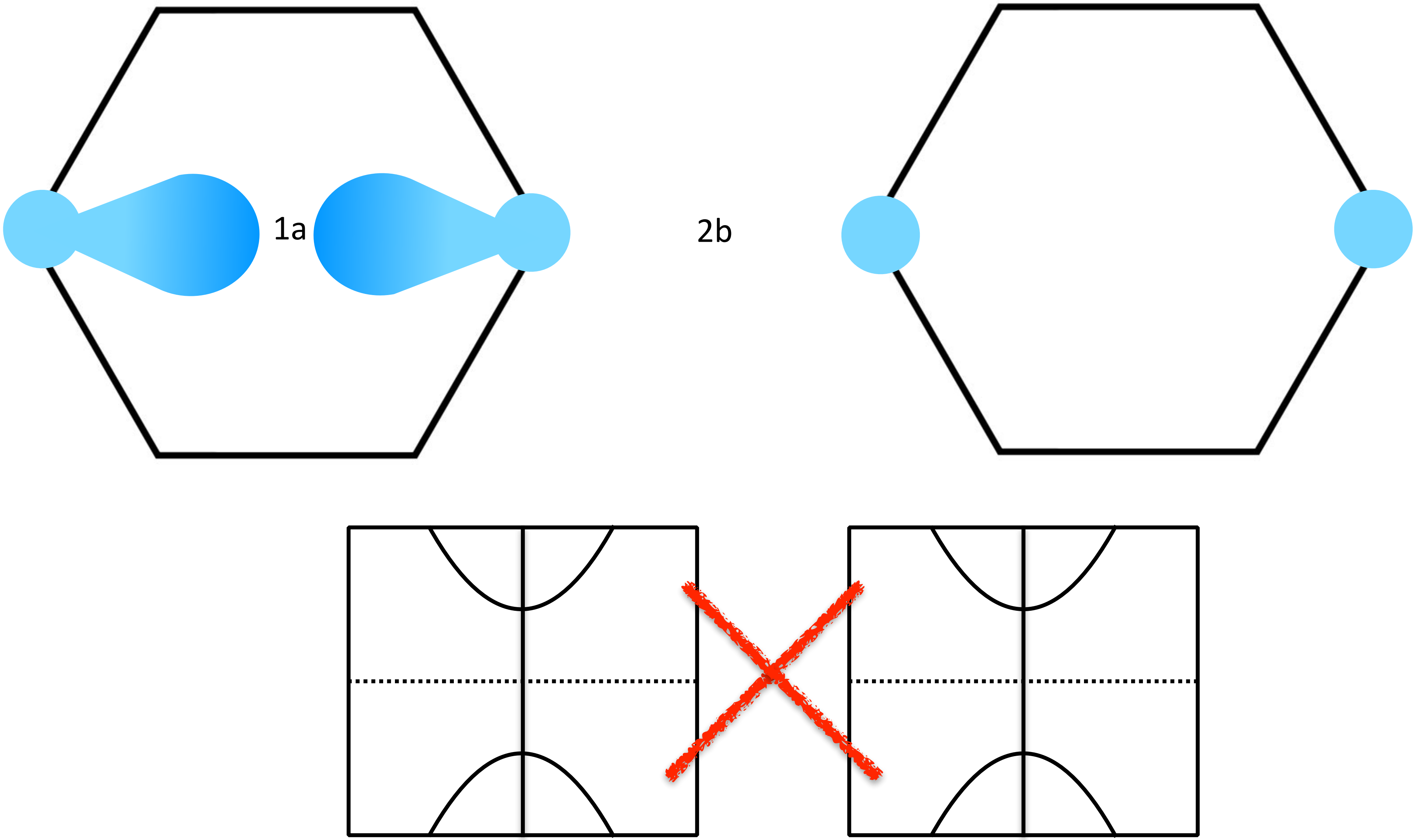
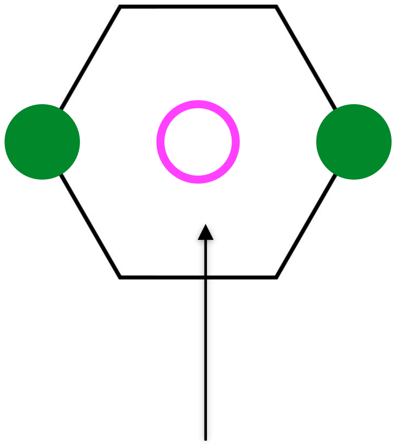
-2
-3
-4
X
Γ
R
M
Γ
X
M
-X2-X5
-Γ6-Γ7
-X3-X4
-R7-R7
-R4-R4
-Γ6-Γ7
-M5-M5
-M5-M5

Obstructed atomic insulators



Obstructed atomic insulators

Symmetry data vector : b=$\sum_l n_i(\mathbf{k}) = \sum_m a_m \mathrm{EBR}$ { EBR1, EBR2



Obstructed Wannier Charge Center

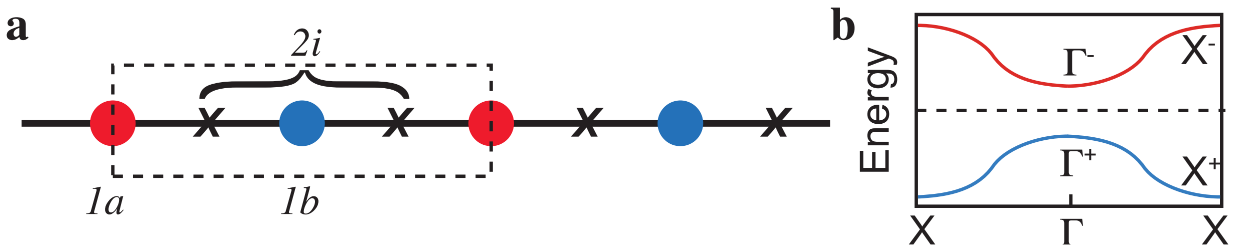
Y. Xu et al arXiv:2106.10276, Z. Song et al. Science 367 (2020)

Obstructed atomic insulators

SSH chain in P-1

(1) 2i sites occupied by atoms
Insulating state: N_e even

(3) Ne=4n+2 -> **BR** of **dim 2** is needed



(2) **dim** of BR at 2i is **4**

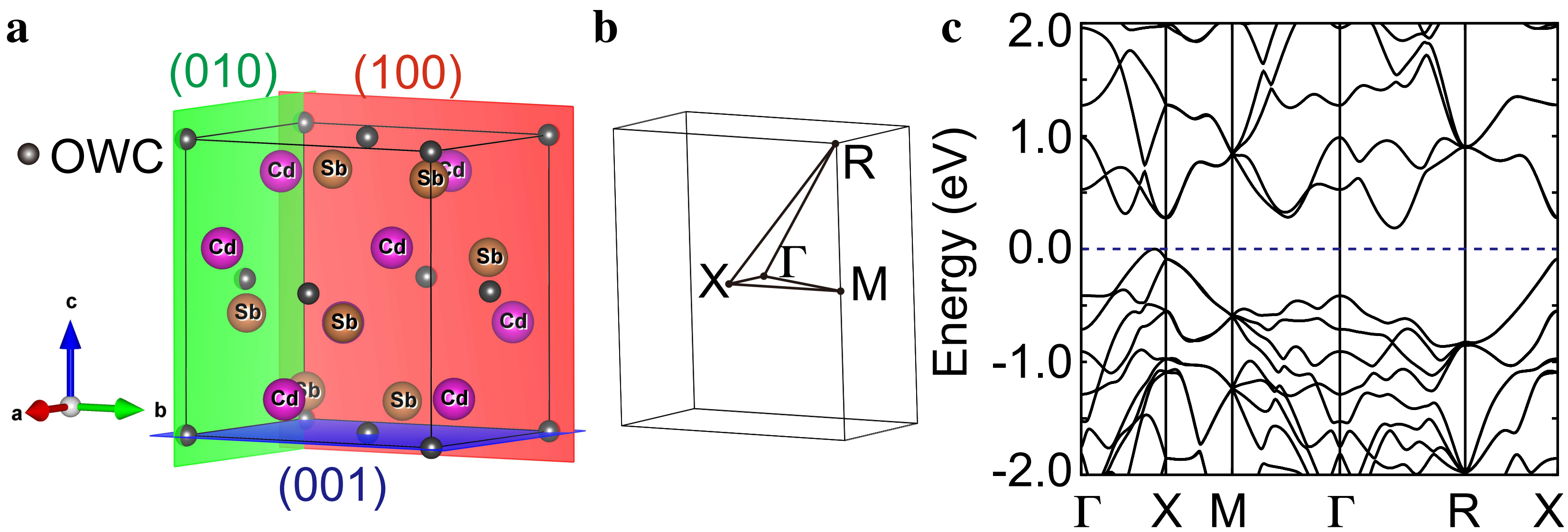
OWCC sitting at 1a

Y. Xu et al arXiv:2106.10276

Obstructed atomic insulators

CdSb in Pbca (No. 61)

Cleavage cuts the OWCC



Cd and Sb both in 8c Wyckoff position

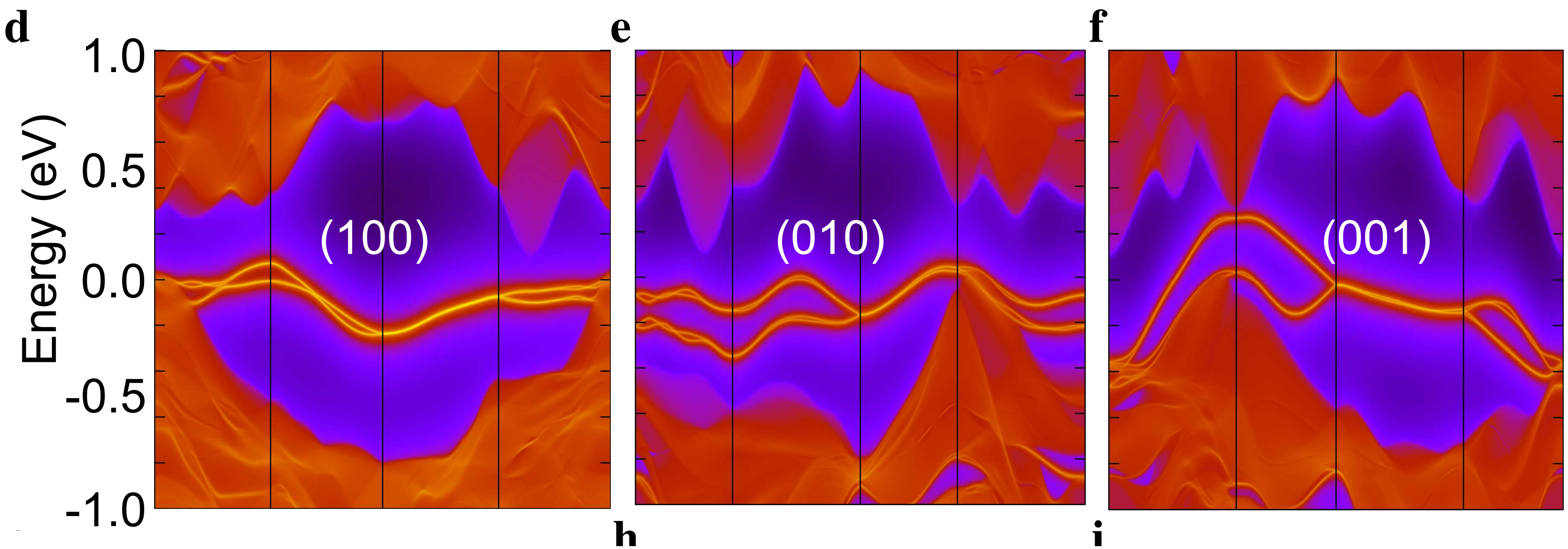
$N_e = 56$

Y. Xu et al arXiv:2106.10276

Obstructed atomic insulators

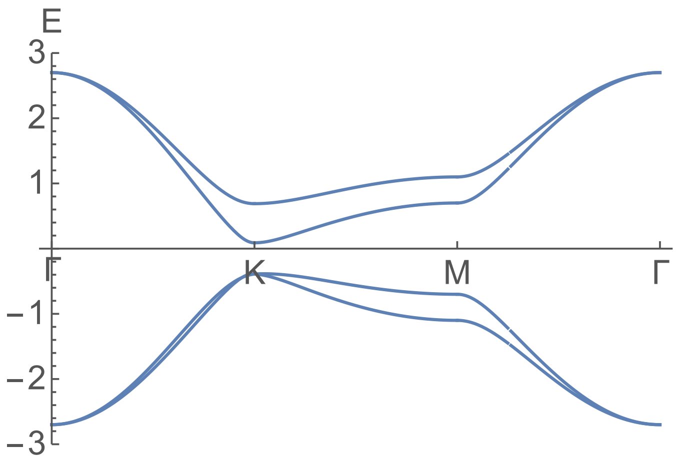
CdSb in Pbca (No. 61)

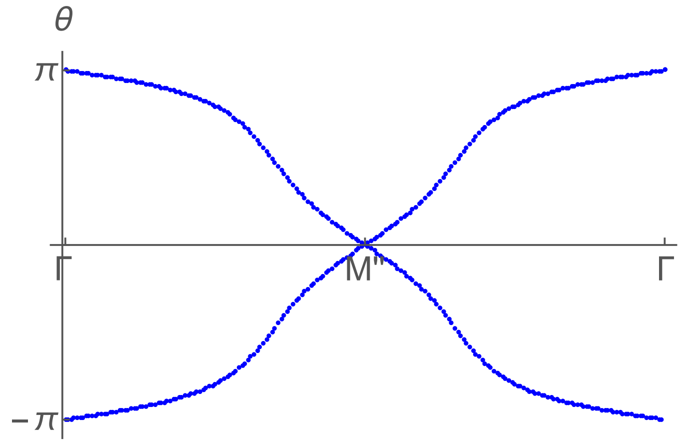
Cleavage cuts the OWCC



Y. Xu et al arXiv:2106.10276

Topological Fragile Phase



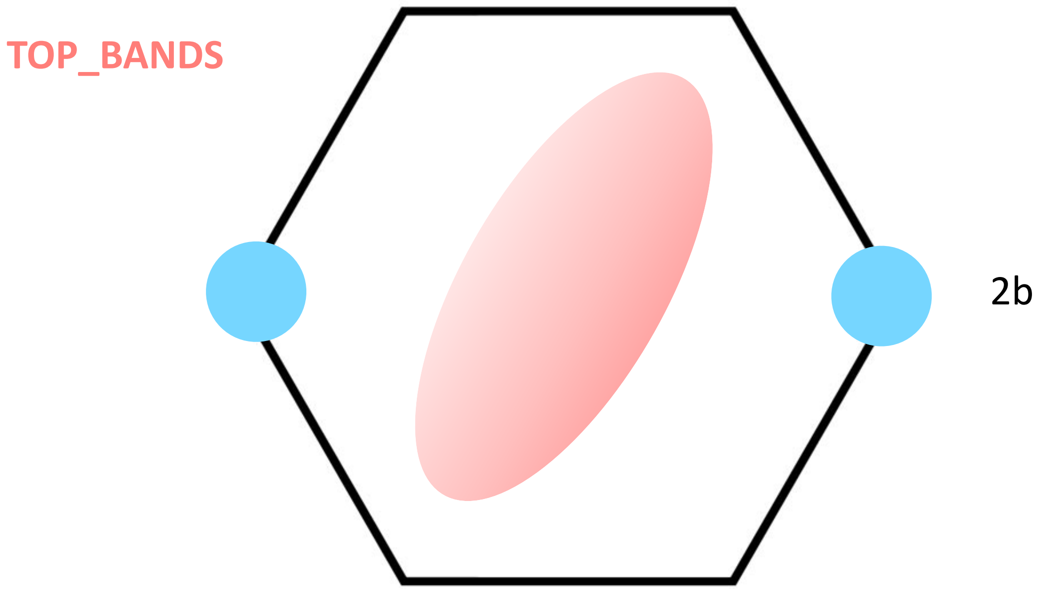


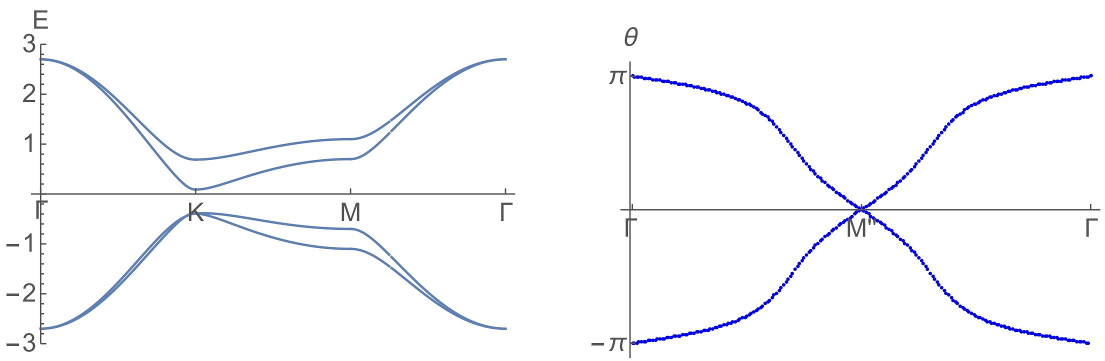
EBR induced at 2b = **TOP_BANDS** **+ EBR induced at 1a (OAL)**

Fragile: EBR_F=**EBR1**-EBR2

Phys. Rev. Lett. 120, 266401 (2018)

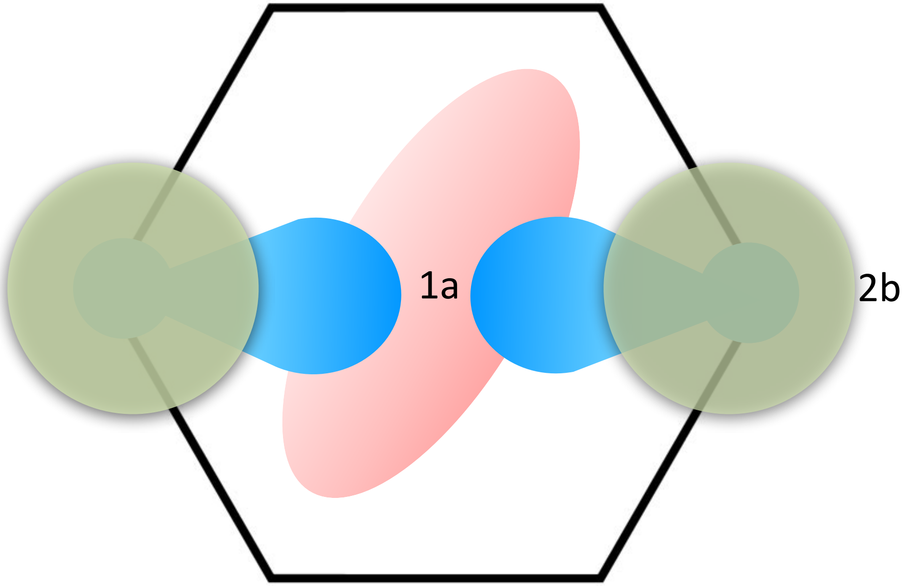
Topological Fragile Phase





Phys. Rev. Lett. 120, 266401 (2018)

Topological Fragile Phase



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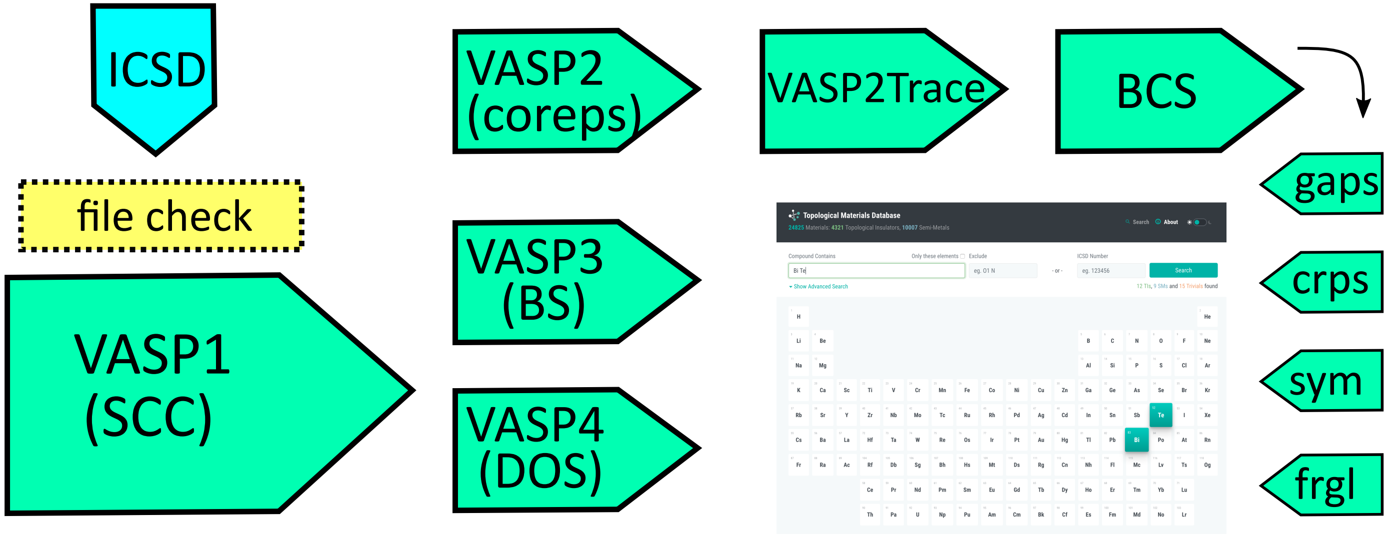
Phys. Rev. Lett. 120, 266401 (2018)

Topological Quantum Chemistry



Nature (2019)

Topological Quantum Chemistry

2019 TQC (2 years)
~10k topological materials

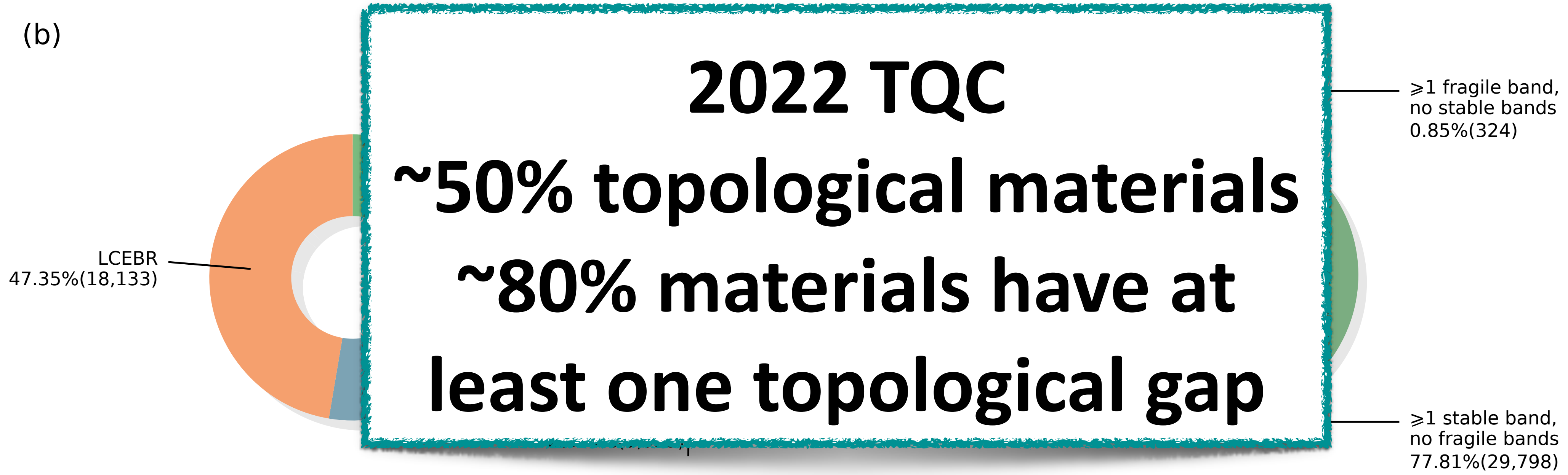
Nature (2019)

All gaps in the energy spectrum

Topology at E_F

Topology at any filling

(b)



2022 TQC

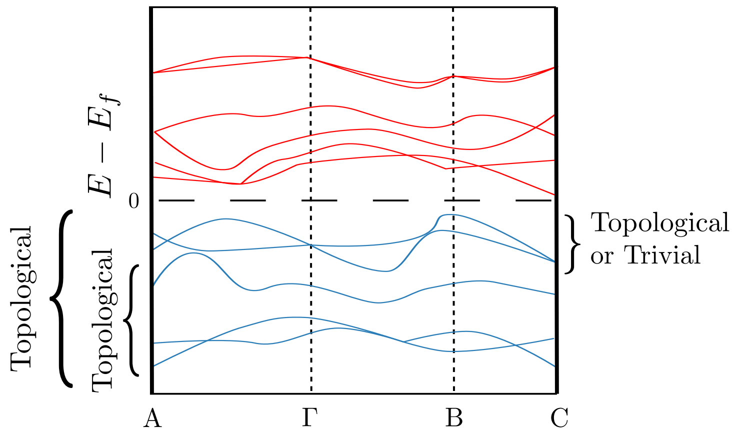
~50% topological materials

~80% materials have at least one topological gap

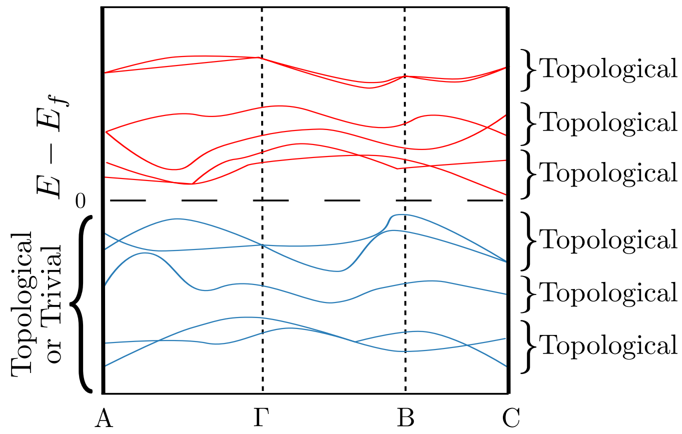
Science 376 (6595) (2022)

All gaps in the energy spectrum

Repeated Topology

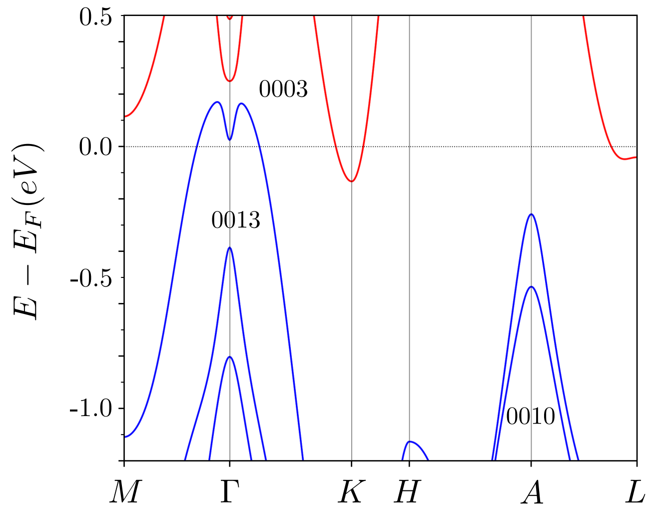


Super Topology

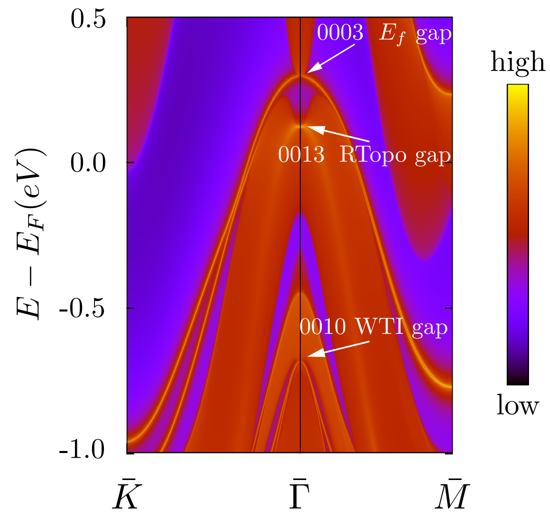


Bi_2Mg_3 - ICSD 659569 - SG 164 ($P\bar{3}m1$) - SEBR

$Z_{2,1} = 0$ $Z_{2,2} = 0$ $Z_{2,3} = 0$ $Z_4 = 3$



(0001)-Surface Spectrum of Bi_2Mg_3



Science 376 (6595) (2022)

Magnetic topological insulators

Magnetic co-representations ✅

BCS Applications Implemented for MTQC		
Application	Contents	Description
MKVEC	Momentum stars of the MSGs	SA D1
Corepresentations	Small and full magnetic (co)reps	SA D2
MCOMPREL	Compatibility relations in the MSGs	SA D3
CorepresentationsPG	Magnetic site-symmetry group (co)reps	SA E1
MSITESYM	Magnetic small (co)reps at one **k** point induced from a site **q**	SA E2
MBANDREP	MEBRs of the MSGs	SA E3

Magnetic codes ✅

MAGVASP2TRACE

Magnetic Topological Classification ✅

SSGs (1651)	Type-I MSGs (230)	Type-II SGs (230)	Type-III MSGs (674)	Type-IV MSGs (517)
(Co)reps	✓	✓	✓	✓
Compatibility rel.	✓	✓	✓	✓
EBRs	✓	✓	✓	✓
Enforced SMs	✓	✓	✓	✓
SI group	✓	✓	✓	✓
SI formulas	✓	✓	✓	✓
Fragile criteria		✓		
Stable invariants	*	✓	*	*
Boundary states	*	✓	*	*
SI → invariants	✓	✓	✓	✓

Nature 586 (2020)

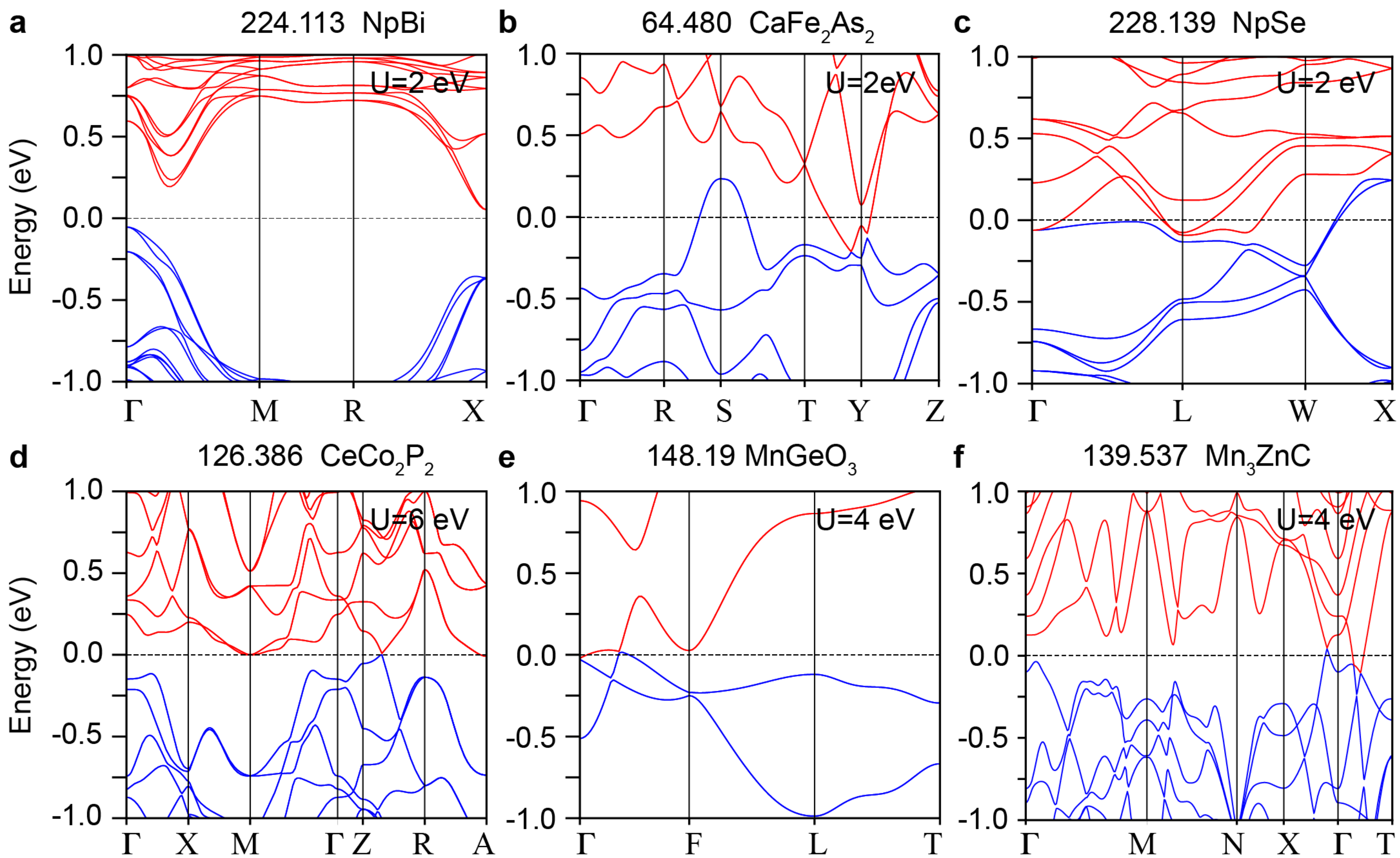
Magnetic topological insulators

First Principles Calculations: 103 materials with non trivial topology

Categories	Properties	Materials
I-A	Non-collinear Manganese compounds	Mn_3GaC, Mn_3ZnC, Mn_3CuN, Mn_3Sn, Mn_3Ge, Mn_3Ir, Mn_3Pt, Mn_5Si_3
I-B	Actinide Intermetallic	$UNiGa_5$, $UPtGa_5$, $NpRhGa_5$, $NpNiGa_5$
I-C	Rare earth intermetallic	$NdCo_2$, $TbCo_2$, $NpCo_2$, PrAg DyCu, NdZn, TbMg, NdMg, Nd_5Si_4, Nd_5Ge_4, Ho_2RhIn_8, Er_2CoGa_8, Nd_2RhIn_8, Tm_2CoGa_8, Ho_2RhIn_8, $DyCo_2Ga_8$, $TbCo_2Ga_8$, Er_2Ni_2In, $CeRu_2Al_{10}$, $Nd_3Ru_4Al_{12}$, $Pr_3Ru_4Al_{12}$, $ScMn_6Ge_6$, YFe_4Ge_4, $LuFe_4Ge_4$, $CeCoGe_3$
II-A	Metallic Iron pnictides	LaFeAsO, $CaFe_2As_2$, $EuFe_2As_2$, $BaFe_2As_2$, Fe_2As, $CaFe_4As_3$, LaCrAsO, Cr_2As, CrAs, CrN
II-B	Semiconducting manganese pnictides	$BaMn_2As_2$ $BaMn_2Bi_2$, $CaMnBi_2$, $SrMnBi_2$, $CaMn_2Sb_2$, CuMnAs, CuMnSb, Mn_2As
II-C	Rare earth intermetallic compounds with the composition 1:2:2	$PrNi_2Si_2$, $YbCo_2Si_2$, $DyCo_2Si_2$, $PrCo_2P_2$, $CeCo_2P_2$, $NdCo_2P_2$, $DyCu_2Si_2$, $CeRh_2Si_2$, UAu_2Si_2, U_2Pd_2Sn, U_2Pd_2In, U_2Ni_2Sn, U_2Ni_2In, U_2Rh_2Sn
II-D	Rare earth ternary compounds of the composition 1:1:1	CeMgPb, PrMgPb, NdMgPb, TmMgPb
III-A	Semiconducting Actinides/Rare earth Pnictides	HoP, UP, UP_2, UAs, NpS, NpSe, NpTe, NpSb, NpBi, U_3As_4, U_3P_4
III-B	Metallic oxides	Ag_2NiO_2, $AgNiO_2$, $Ca_3Ru_2O_7$, Double perovskite Sr_3CoIrO_6
III-C	Metal to insulator transition compounds	NiS_2, $Sr_2Mn_3As_2O_2$
III-D	Semiconducting and insulating oxides, borates, hydroxides, silicates, phosphate	$LuFeO_3$, $PdNiO_3$, $ErVO_3$, $DyVO_3$, $MnGeO_3$, $Tm_2Mn_2O_7$, $Yb_2Sn_2O_7$, $Tb_2Sn_2O_7$, $Ho_2Ru_2O_7$, $Er_2Ti_2O_7$, $Tb_2Ti_2O_7$, $Cd_2Os_2O_7$, $Ho_2Ru_2O_7$, Cr_2ReO6, $NiCr_2O_4$, MnV_2O_4, Co_2SiO_4, Fe_2SiO_4, $PrFe_3(BO_3)_4$, $KCo_4(PO_4)_3$, $CoPS_3$, $SrMn(VO_4)(OH)$, $Ba_5Co_5ClO_{13}$, FeI_2

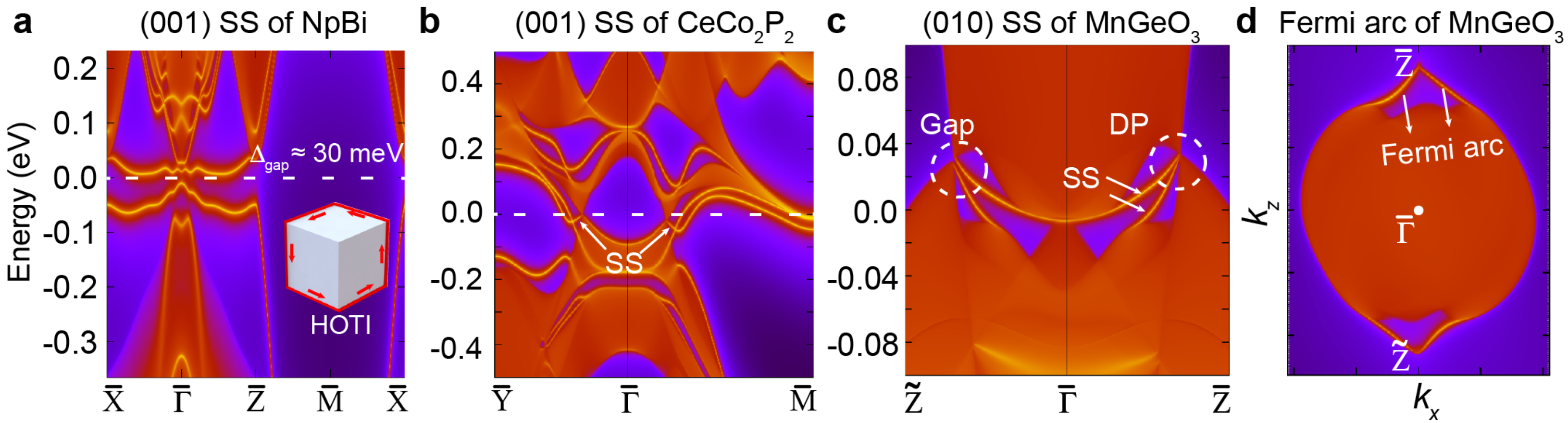
Nature 586 (2020)

Magnetic topological insulators



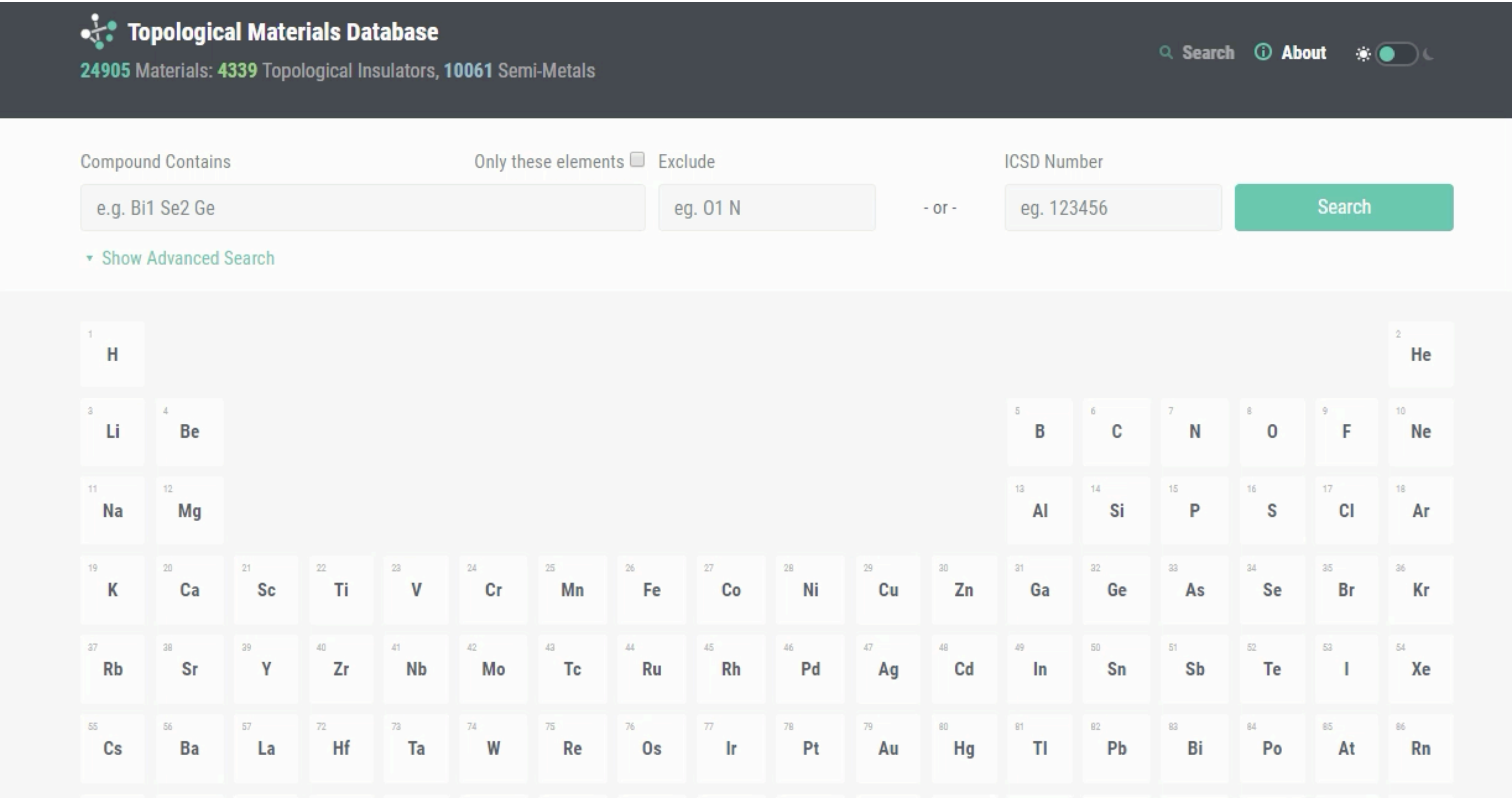
Nature 586 (2020)

Magnetic topological insulators



Topological Materials Database

https://www.topologicalquantumchemistry.org



http://www.cryst.ehu.es/

MAX PLANCK INSTITUTE
FOR CHEMICAL PHYSICS OF SOLIDS

FCT/ZTF

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Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

Structure Utilities

Topological Quantum Chemistry

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

bilbao crystal lographic server

Crystallography Online: Workshop on the use of the structural and magnetic tools of the Bilbao Crystallographic Server
September 2021, Leioa (Spain)

Forthcoming schools and workshops

News:

- **New Article in Nature**
  10/2020: Xu *et al.* "High-throughput calculations of magnetic topological materials" *Nature* (2020) **586**, 702-707.
- New programs: **MBANDREP**, **COREPRESENTATIONS**, **COREPRESENTATIONS PG**, **MCOMPREL**, **MSITESYM**, **MKVEC**, **Check Topological Magnetic Mat**
  10/2020: new tools in the sections "Magnetic Symmetry and Applications" and "Representations and Applications".
  More info
- New section: **TOPOLOGICAL QUANTUM CHEMISTRY**
  10/2020: tools for the identification of the

Quick access to some tables

Space Groups
Plane Groups
Layer Groups
Rod Groups
Frieze Groups
2D Point Groups
D Point Groups
agnetic Space Groups

Public codes

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FOR CHEMICAL PHYSICS OF SOLIDS

Bilbao Crystallographic Server → Check Topological Mat. Help

Check Topological Mat

Check Topological Mat.

Given a file that contain the eigenvalues at each maximal k-vec of a space group, the program gives the set of irreducible representations at each maximal k-vec (time-reversal is assumed). Then, using the compatibility relations and the set of Elementary Band Representations (EBRs), it checks whether the set of bands can be put as linear combinations of EBRs. This (self-explanatory) file shows the format of the file to be uploaded in the menu on the right:

File_Description

You can download examples of input files here:

Example_Ag1Ge1Li2 Example_Ag1O2Sc1
Example_B2Ca3Ni7 Example_of_Bad_File
Example_Ba3Ca1O9Ru2

You can generate the "trace.txt" file in your own computer using VASP and this program (fo

vasp2trace

Read the "README.pdf" file for help on the use of vasp2trace.

Alternatively, you can use the irvsp package.

If you are using "Check Topological Mat." and/or "vasp2trace" programs in the preparation
cite this reference:

M.G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B.A. Bernevig, Z. Wang Nature(2019) 56
doi:10.1038/s41586-019-0954-4

Link to the catalogue of topological materials,

www.topologicalquantumchemistry.com

Upload your traces.txt file (see the help in the column on the left).

Browse... No file selected.

Show

https://irrep.dipc.org

IRREP

Search docs

- Installation
- Organizations
- External software used
- People
- Index

» IrRep

IRREP

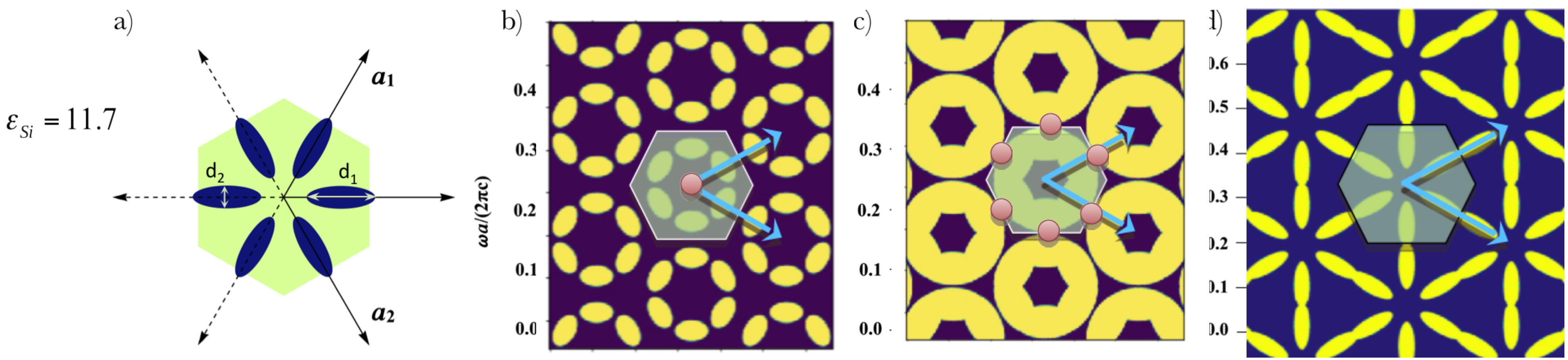
is a code to calculate symmetry eigenvalues of electronicBloch states in crystalline solids and the irreducible representations under which they transform. It can receive as input bandstructures computed with VASP, Abinit, Quantum Espresso or any code with an interface to Wannier90.

Characteristics

- **Any space group** - It can be applied to bandstructures of crystals in any of the **230** space groups preserving **time-reversal** symmetry.
- **spinful or spinless** - It includes both, **single** (spinless) and **double-valued** (spinful) groups. Also, it accepts calculations with **spin-orbit coupling** corrections.
- **Any unit cell** - Bandstructures calculated with any choice of the unit cell are welcome: primitive, conventional,...
- A `trace.txt` file that can be passed directly to CheckTopologicalMat is generated.
- Adding interfaces to other DFT codes is easy. You are welcome!

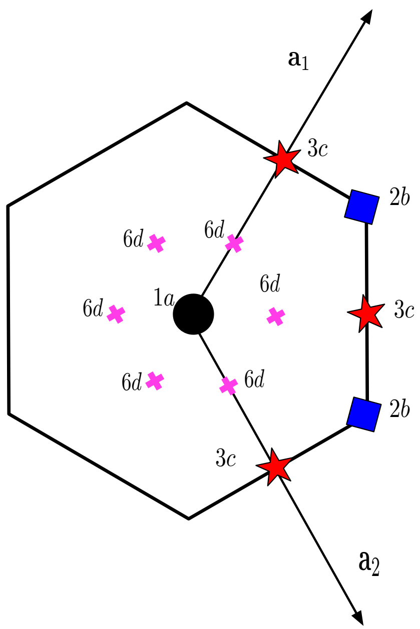
M. Iraola Com. Phys. (2022)

Topological Photonic Crystals in 2D



MPB computed bands, GTPack computed representations

S. G. Johnson and J. D. Joannopoulos, Optics express 8, 173 (2001).

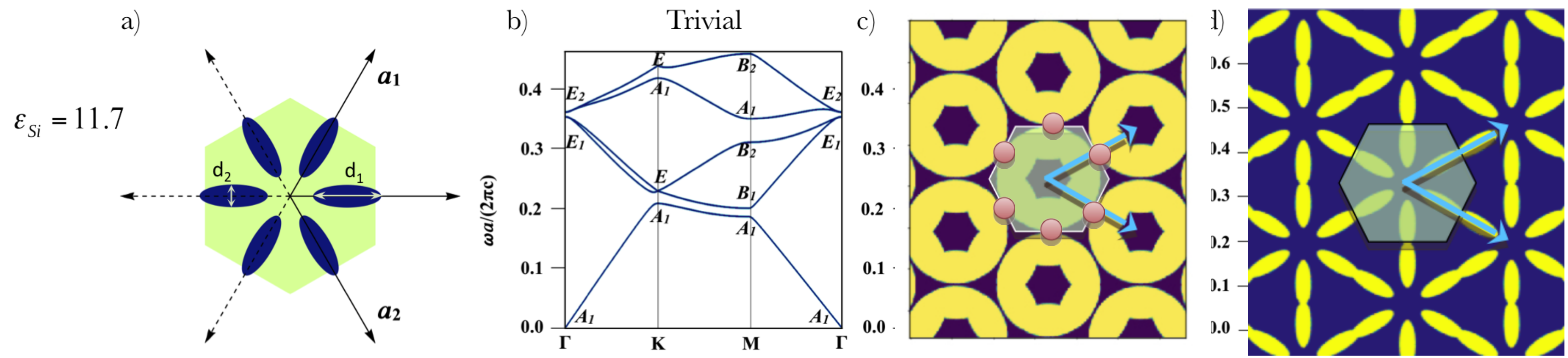


EBR	Γ	K	M
$(A_1 \uparrow G)_{1a}$	A_1	A_1	A_1
$(E_1 \uparrow G)_{1a}$	E_1	E	$B_1 \oplus B_2$
$(A_1 \uparrow G)_{3c}$	$A_1 \oplus E_2$	$E \oplus A_1$	$A_1 \oplus B_1 \oplus B_2$

Haldane and Raghu, PRL (2008), PRA (2008)

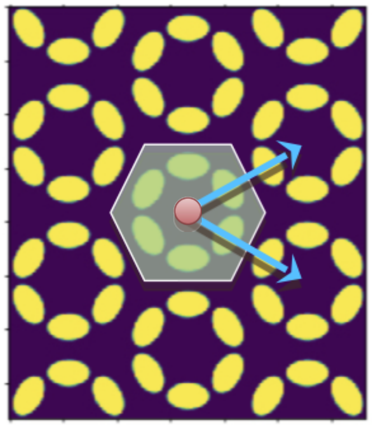
Blanco de Paz, PRR 1, 032005(R), J. Phys.: Condens. Matter **34** 314002, Advanced Quantum Technologies 3 (2), 1900117, Devescovi Nat Commun **12**, 7330 (2021)

Topological Photonic Crystals in 2D



MPB computed bands, GTPack computed representations

$$\nabla \times \left(\frac{1}{\epsilon(\mathbf{r})} \times \mathbf{H}(\mathbf{r}) \right) = \left(\frac{\omega}{c} \right)^2 \mathbf{H}(\mathbf{r})$$



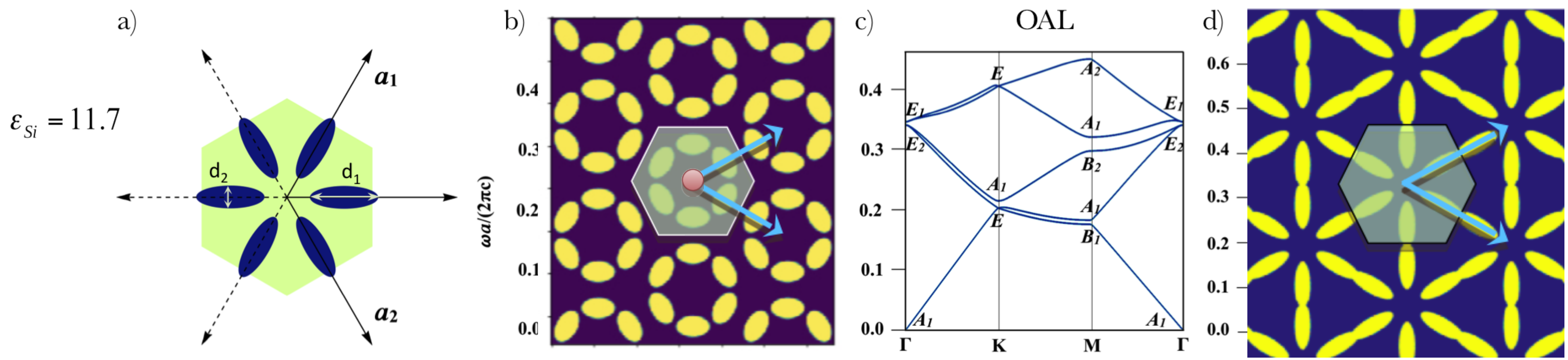
Band Repres.	Γ	K	M
Band 1	A_1	A_1	A_1
Bands 2+3	E_1	E	B_1+B_1

Band 1 → $(A_1 \uparrow G)_{1a}$

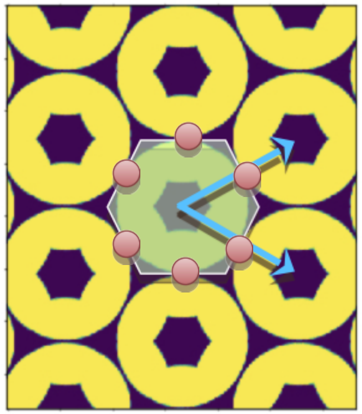
Bands 2+3 → $(E_1 \uparrow G)_{1a}$

Blanco de Paz, PRR 1, 032005(R), J. Phys.: Condens. Matter **34** 314002, Advanced Quantum Technologies 3 (2), 1900117, Devescovi Nat Commun **12**, 7330 (2021)

Topological Photonic Crystals in 2D



MPB computed bands, GTPack computed representations



Band Repr.	Γ	K	M
Bands 1+2+3	A_1+E_2	A_1+E	$A_1+B_1+B_2$

$\Rightarrow \left(A_1 \uparrow G\right)_{3c}$

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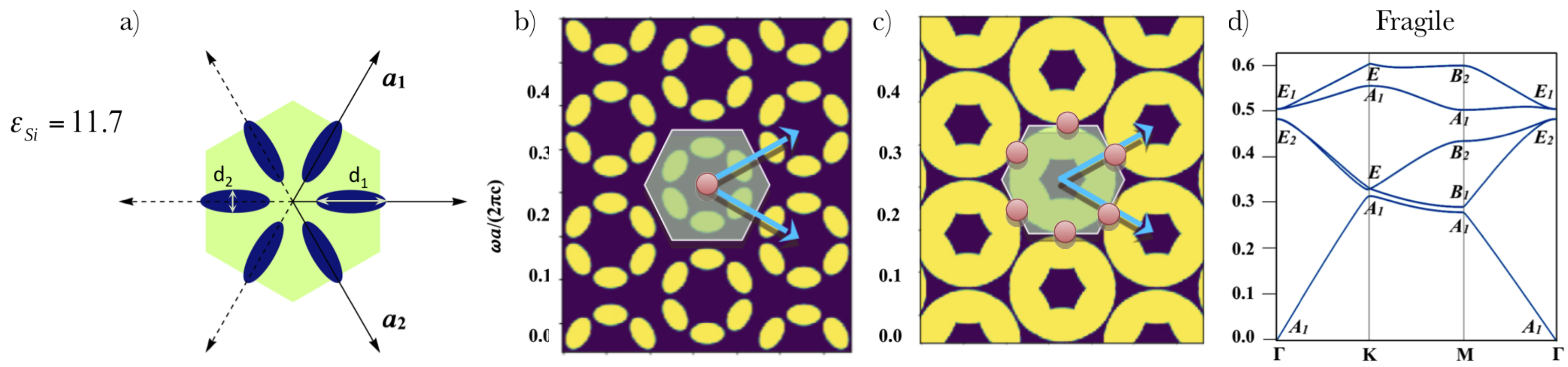
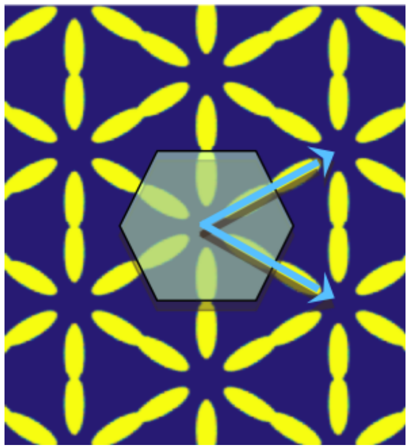
Topological Photonic Crystals in 2D



MPB computed bands, GTPack computed representations



Band Repres.	Γ	K	M
Band 1	A_1	A_1	A_1
Bands 2+3	E_2	E	B_1+B_2

Band 1 → $(A_1 \uparrow G)_{1a}$

Bands 2+3 → ???

$$(A_1 \uparrow G)_{3a} - (A_1 \uparrow G)_{1a}$$

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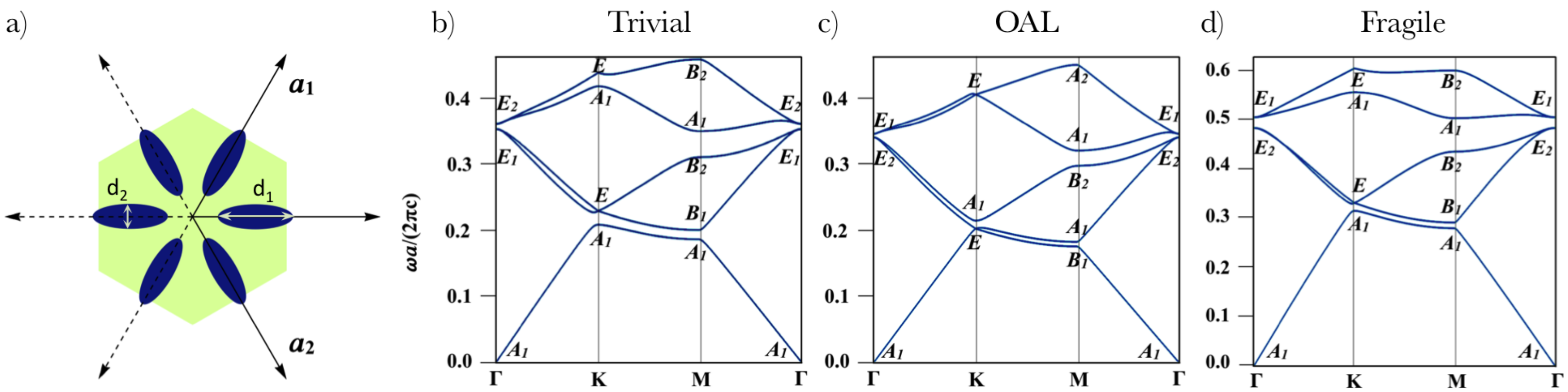
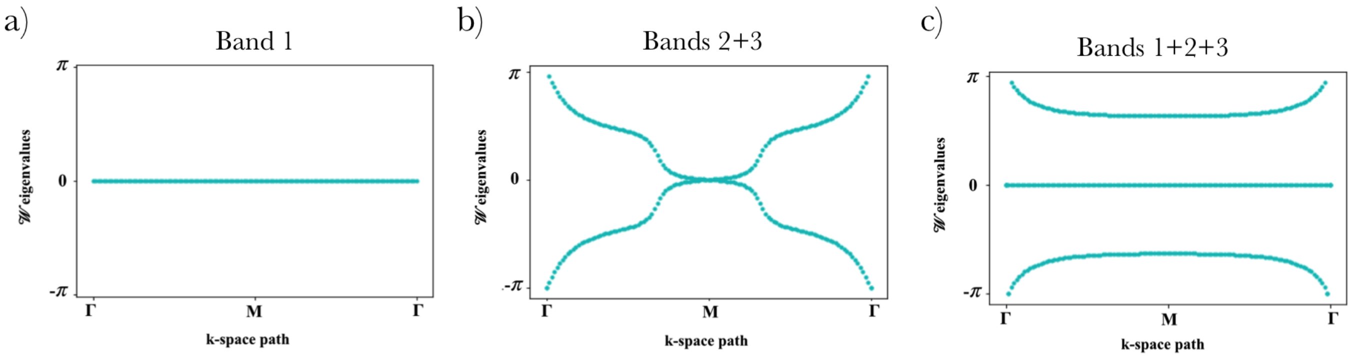
Topological Photonic Crystals in 2D



MPB computed bands, GTPack computed representations

Wilson loops of Fragile phase



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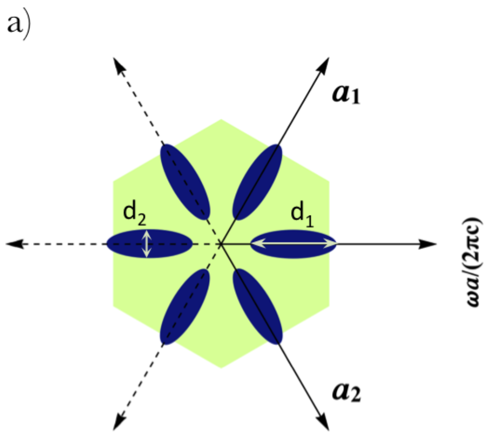
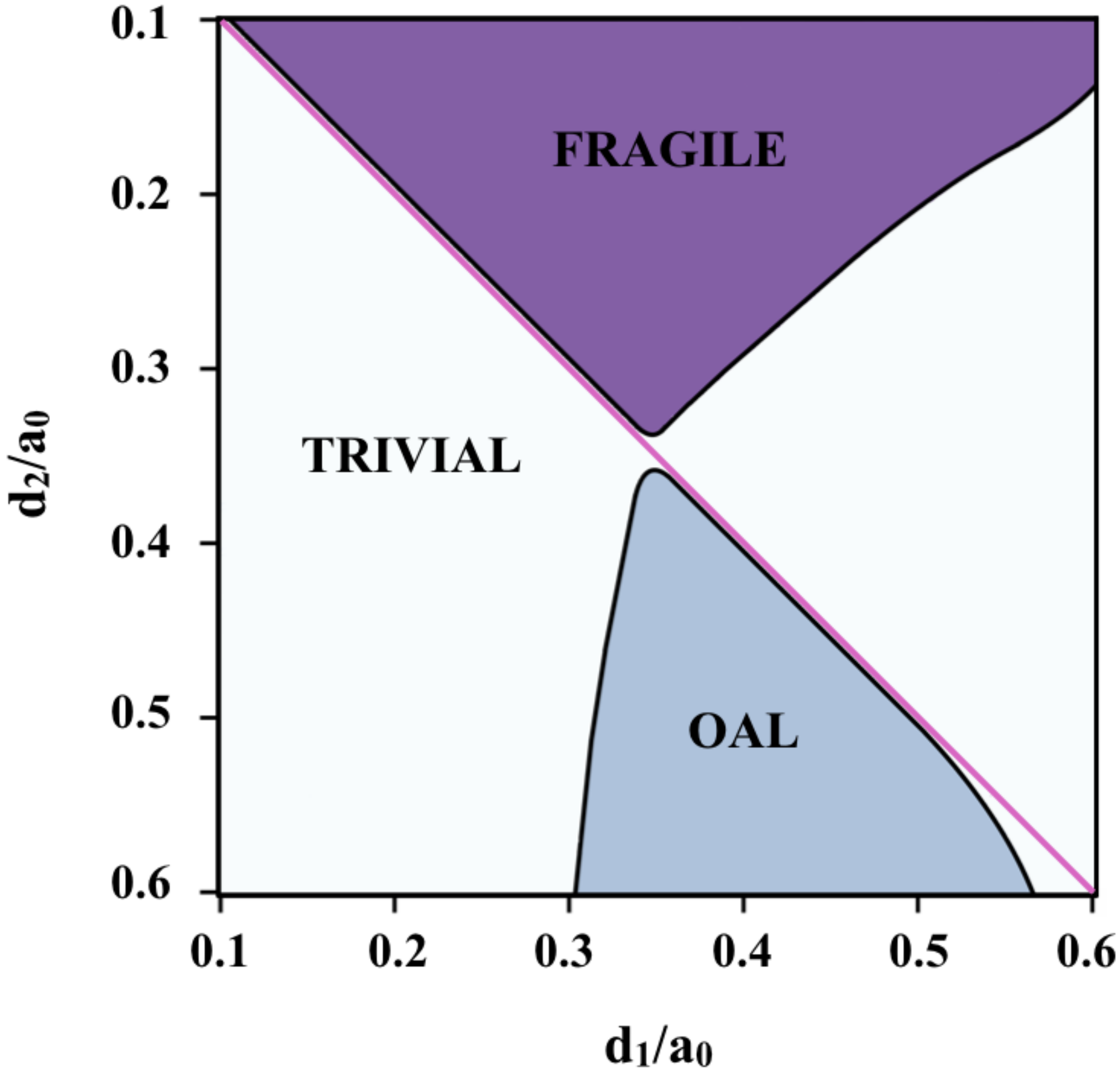
Topological Photonic Crystals in 2D



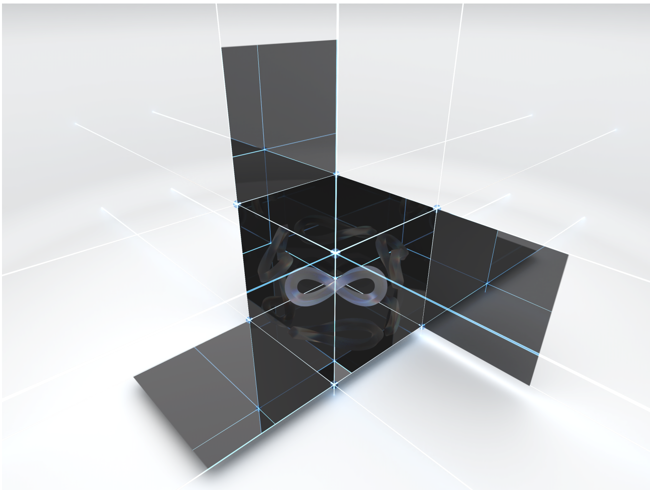


Blanco de Paz, PRR 1, 032005(R), J. Phys.: Condens. Matter **34** 314002, Advanced Quantum Technologies 3 (2), 1900117, Devescovi Nat Commun **12**, 7330 (2021)

Summary and conclusions

Band Topology

- We can claim we have understood band topology very deeply
- Topology was unknown but not a rarity
- High throughput searches for magnetic and non-magnetic materials



Nature Reviews Materials, 1-21 (2021)