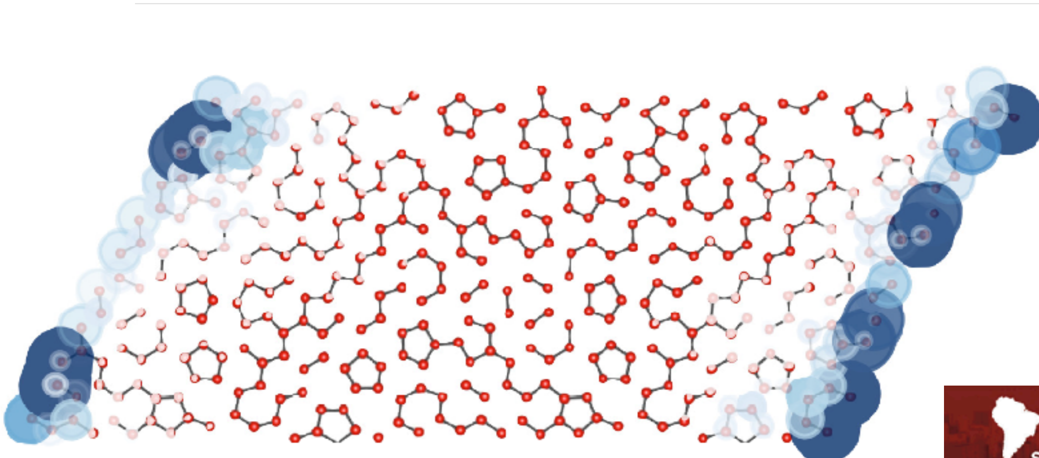
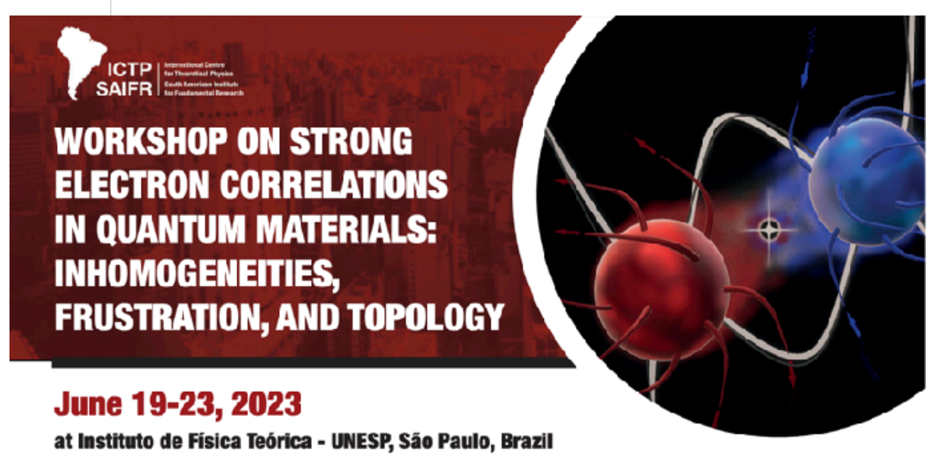
Topological phase transitions in strongly disordered and amorphous systems

Caio Lewenkopf
Universidade Federal Fluminense

INSTITUTO DE FÍSICA
Universidade Federal Fluminense

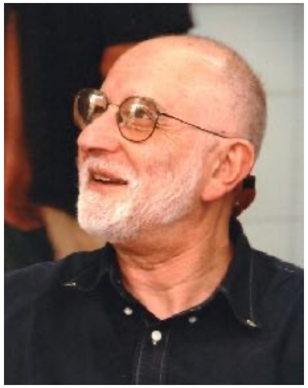




IQHE: Topological formulation

TKNN:
PRB (1982)

$$\sigma_{xy} = \frac{e^2}{h} N$$



M. Berry

D. Thouless
Nobel 2016

Berry curvature (gauge invariant)

Proc R. Soc (1984)

$$H(\xi)\,|\psi(\xi)\rangle = E(\xi)\,|\psi(\xi)\rangle$$

$$\Omega(\xi) = i\Big\langle \nabla_\xi \psi(\xi)\,\Big|\times\Big|\,\nabla_\xi \psi(\xi)\Big\rangle$$

$$N = \frac{1}{2\pi}\int d^2\mathbf{k}\,\Omega(\mathbf{k})$$

integral over a torus:
first Chern number

$$C_1 \equiv \frac{1}{2\pi}\int_{\mathbb{T}^2} f \in \mathbb{Z}.$$

(if not zero) signature
of a topological state

Topological insulators: precursors

Haldane, PRL (1988)

D. Haldane
Nobel 2016

IQH without magnetic field

graphene tight-binding Hamiltonian

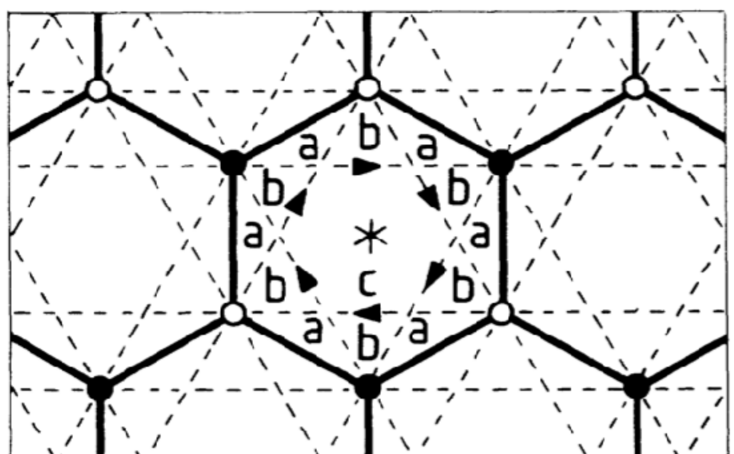
$$H_0 = -t \sum_{\langle i,j \rangle} a_i^\dagger b_j + \mathrm{H.c}$$

mass term:

$$H_1 = M \sum_i \left(a_i^\dagger a_i - b_i^\dagger b_i \right)$$

+ “magic"

$t_2 e^{i\phi}$



Chern insulator

Dirac fermions: topological behaviour

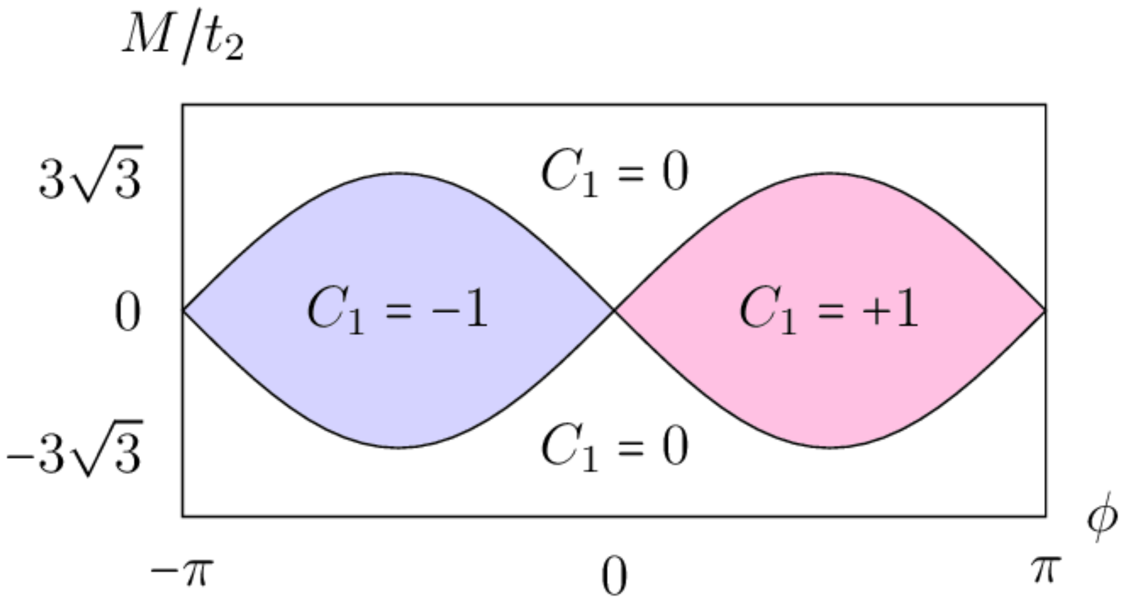
https://topocondmat.org/w4_haldane/haldane_model.html

Chern number

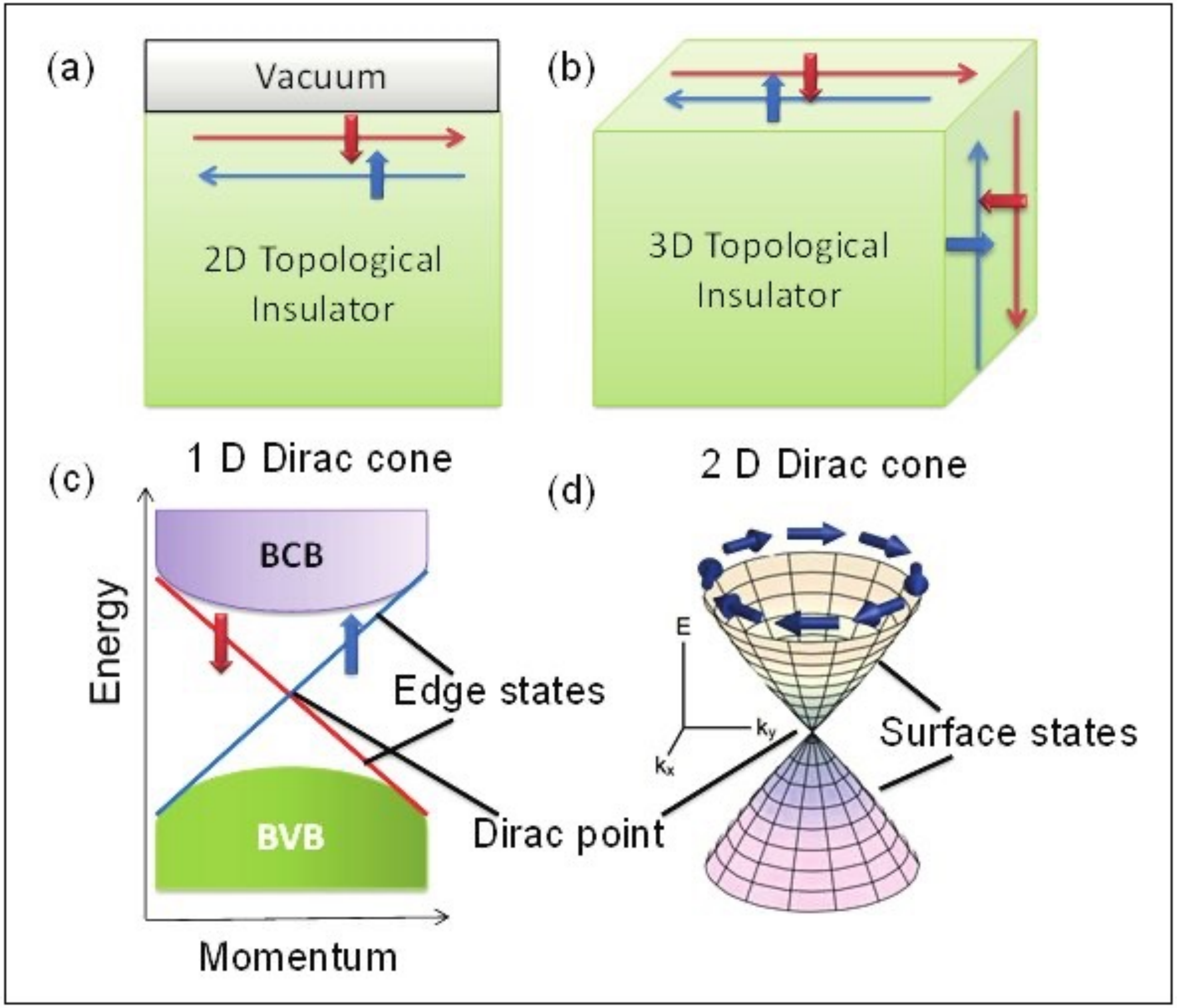
$$C_1 = \frac{1}{2\pi}\int_{\mathrm{BZ}} d^2k\,\Omega(\mathbf{k})$$

Haldane model:

Phase diagram



(Band) Topological Insulators

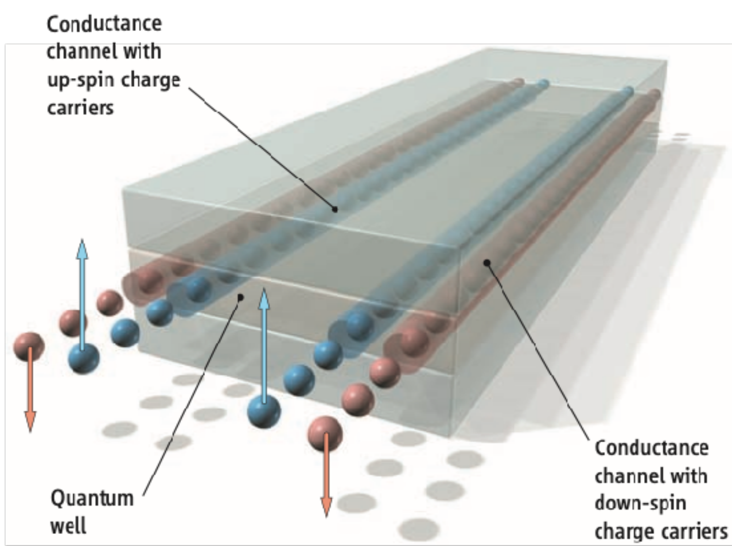


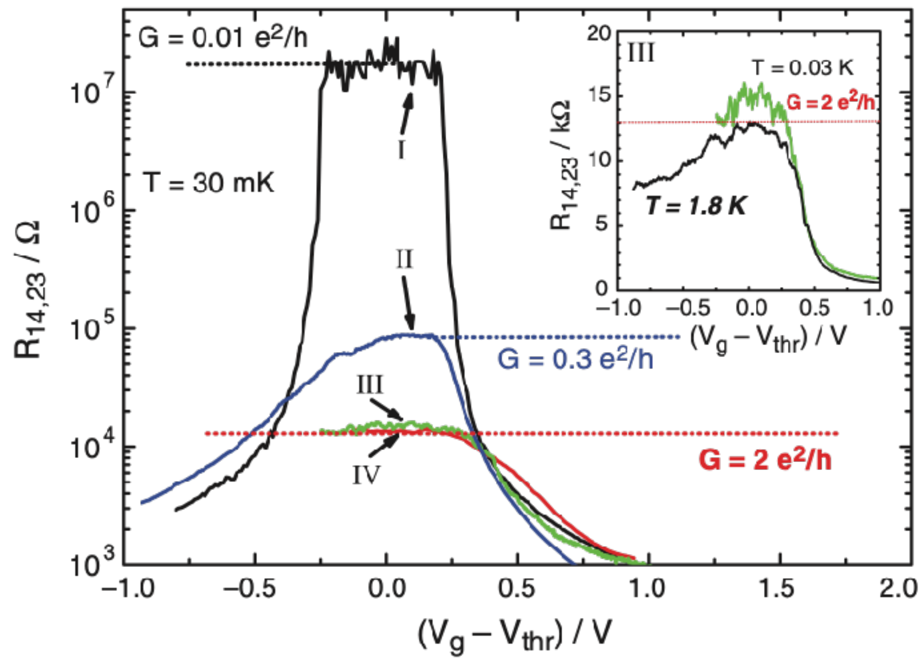
Experiments: 2D topological insulators

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]

Science 2007



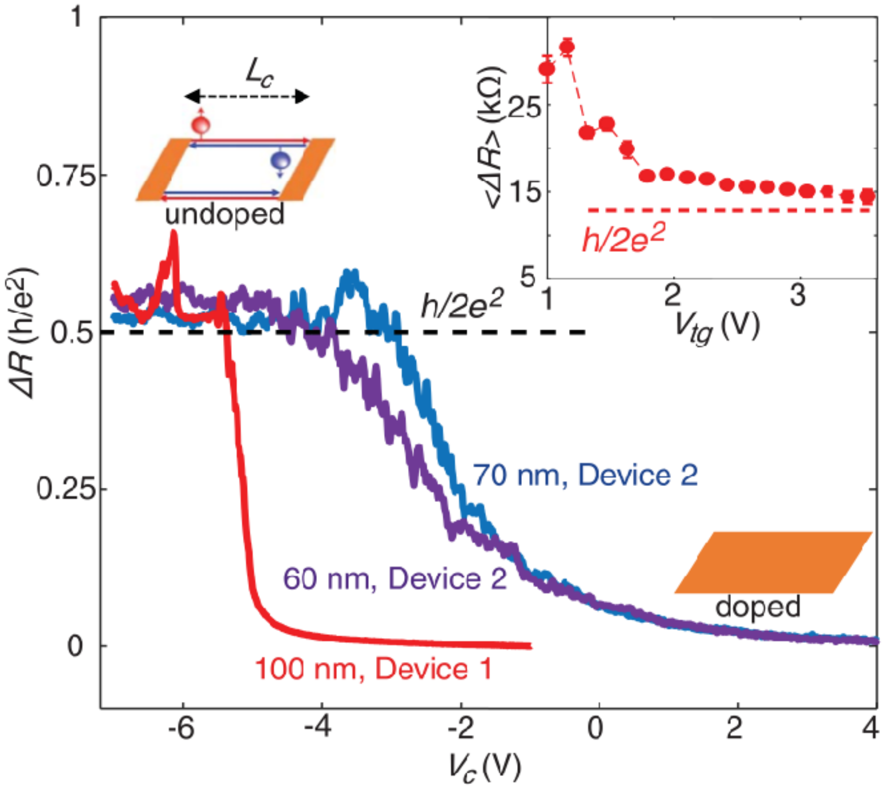


short vs long samples: Gussev et al, PRL (2010), PRB (2011)

Experiments: 2D topological insulators

Material platform: WTe_2

(2D crystal)

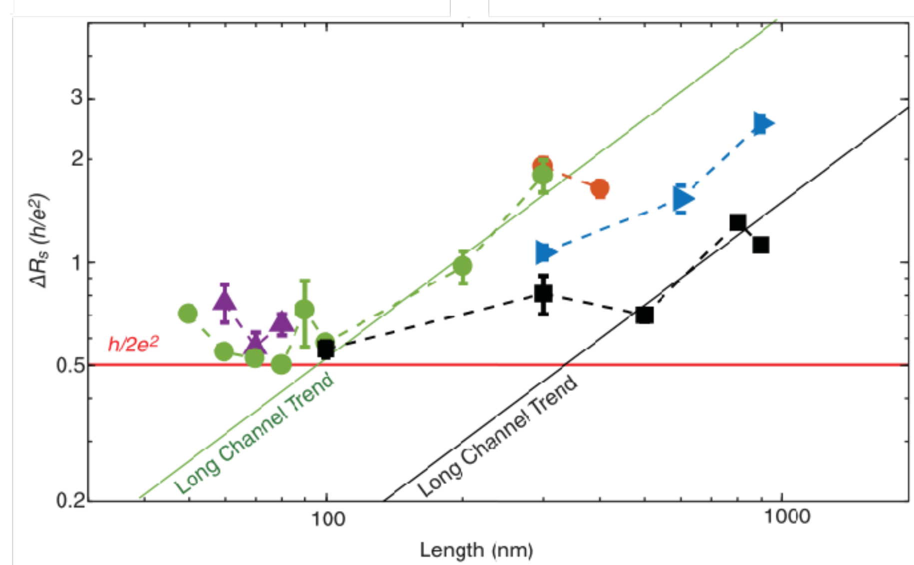


TOPOLOGICAL MATTER

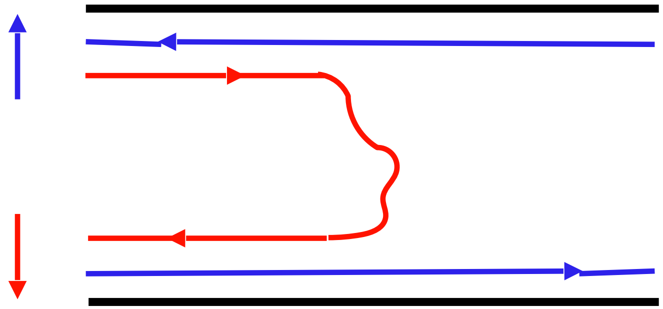
Observation of the quantum spin Hall effect up to 100 kelvin in a monolayer crystal

Sanfeng Wu,[1*†] Valla Fatemi,[1*†] Quinn D. Gibson,[2] Kenji Watanabe,[3] Takashi Taniguchi,[3] Robert J. Cava,[2] Pablo Jarillo-Herrero[1†]

Science **359**, 76–79 (2018)



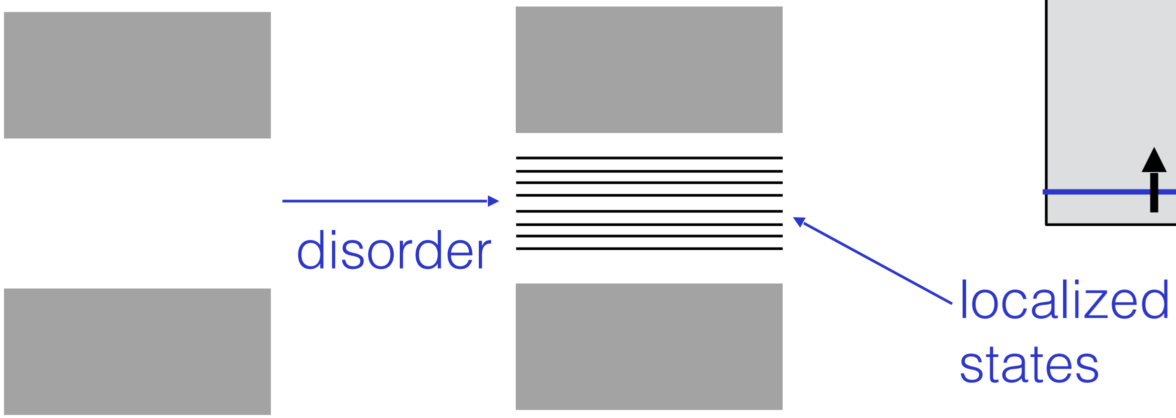
Interedge backscattering

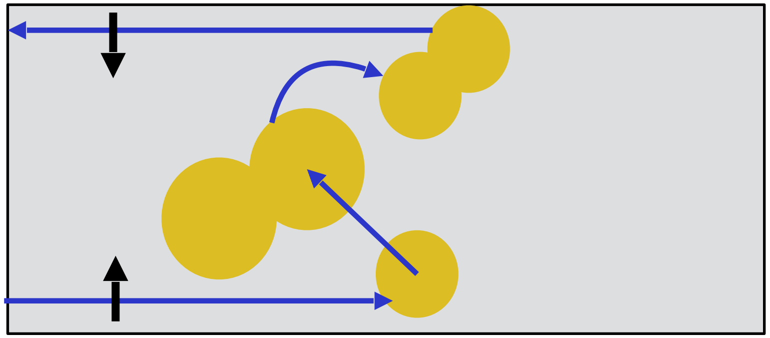


no spin-flip

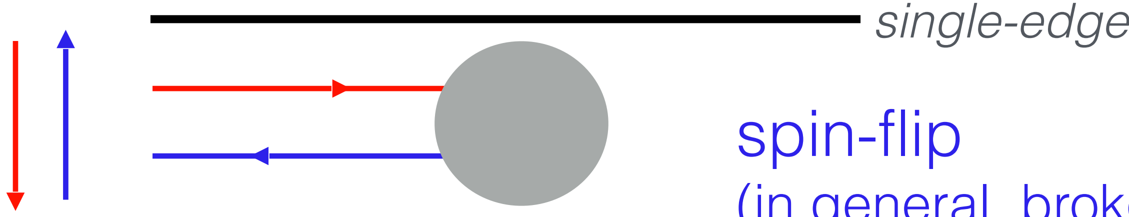
“percolation" mechanism

localization-driven





Intraedge backscattering



spin-flip
(in general, broken time-reversal symmetry)

- magnetic impurities — no! (experimental)
- phonons — no (wrong *T* dependence)
- Rashba spin-orbit coupling — hardly (under discussion)
- charge puddles many-body effects — no (wrong *T* dependence)
- nuclear spins — perhaps (under discussion)
- non-magnetic disorder mechanisms
  (disorder + interactions)

Non-magnetic disorder mechanisms

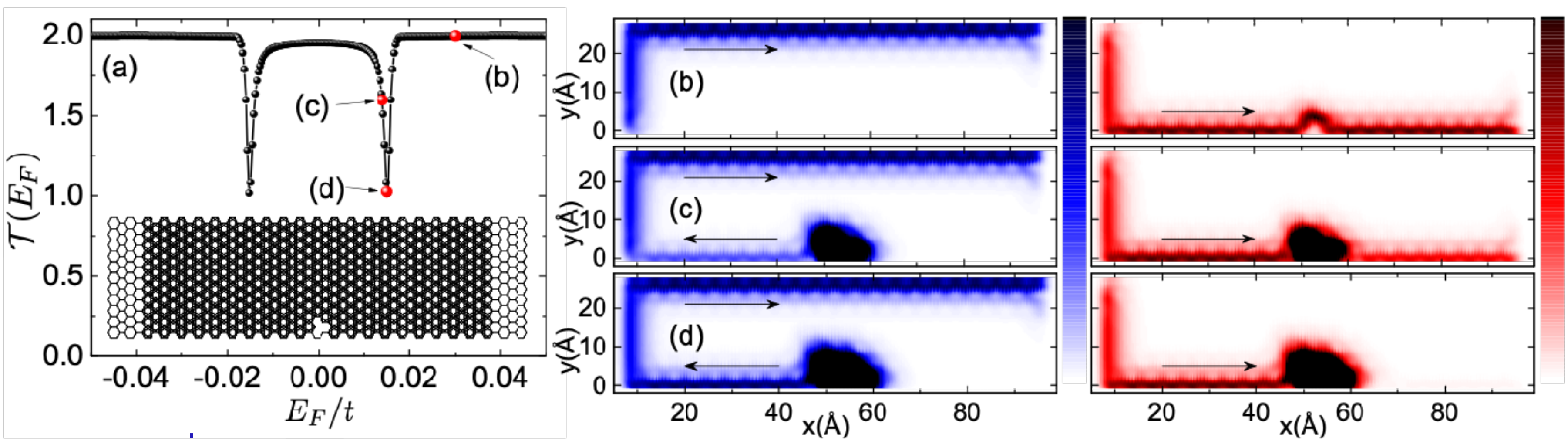
Leandro Lima
(UFRRJ)

PRB (2022)

localization + e-e interactions

↓ Stoner instability

local magnetic moments



vacancies

Model: Kane-Mele + Hubbard mean-field

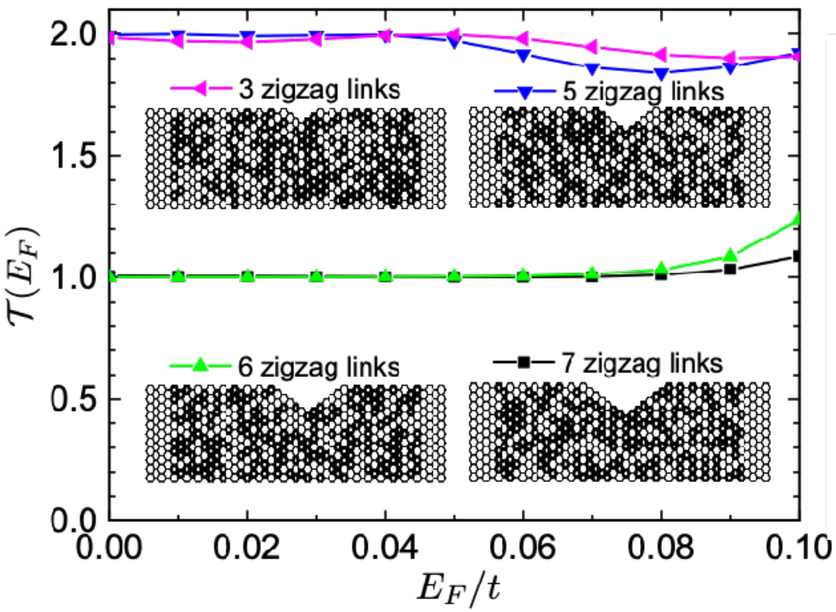
Non-magnetic disorder mechanisms

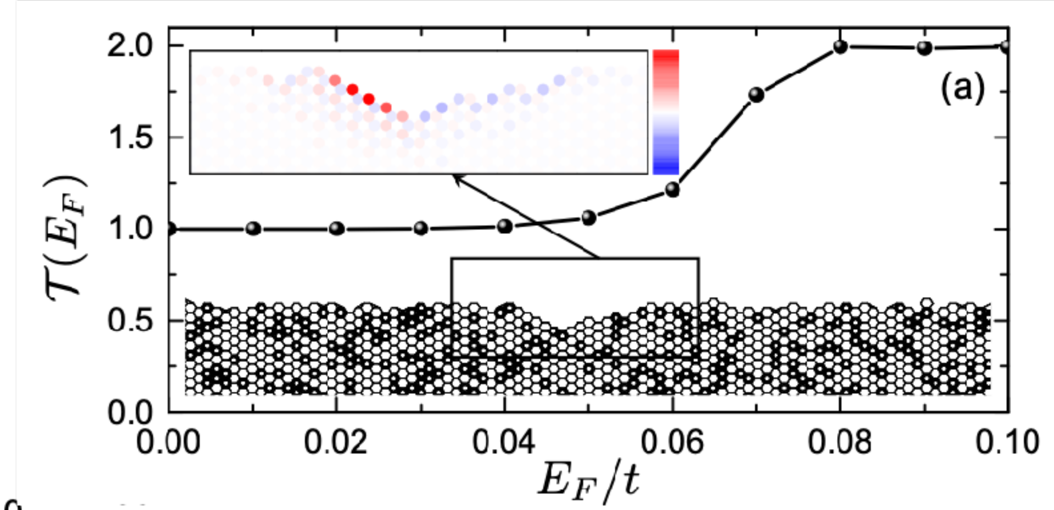
Leandro Lima
(UFRRJ)

localization + e-e interactions

Stoner instability

local magnetic moments





Topological insulators:

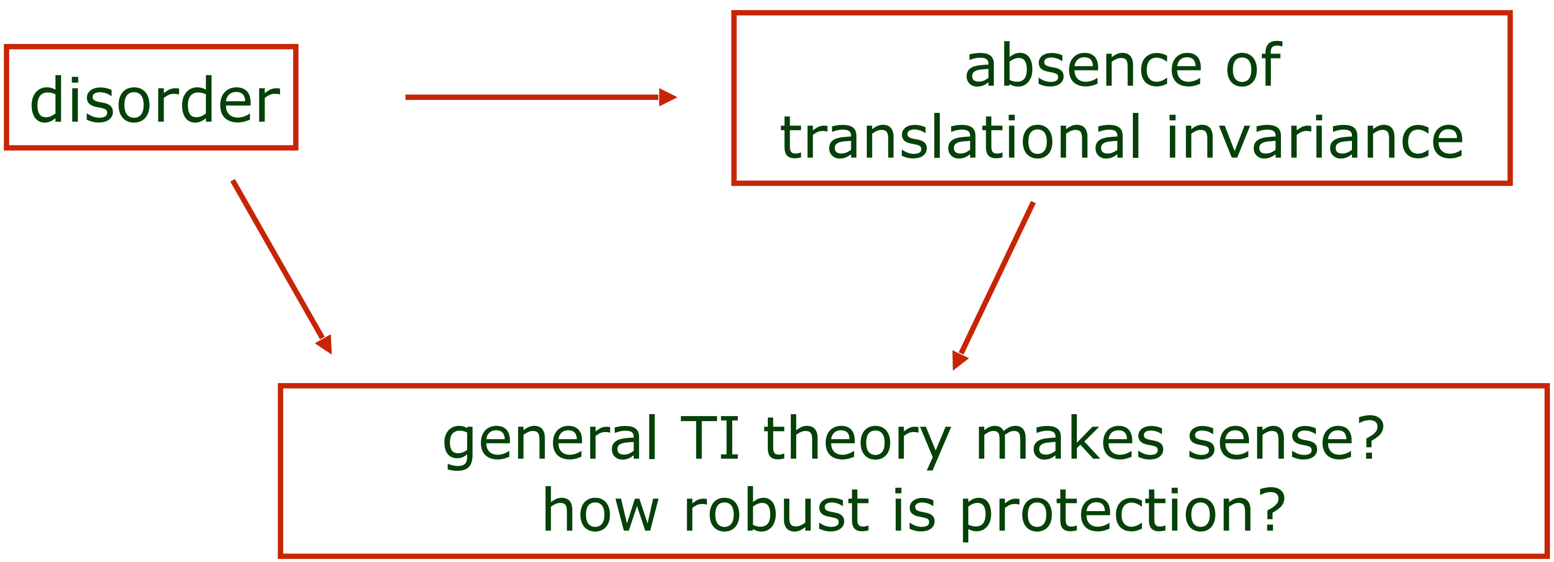
Strong Disorder

Topological insulators: Strong Disorder

theoretical characterization of topological insulators:

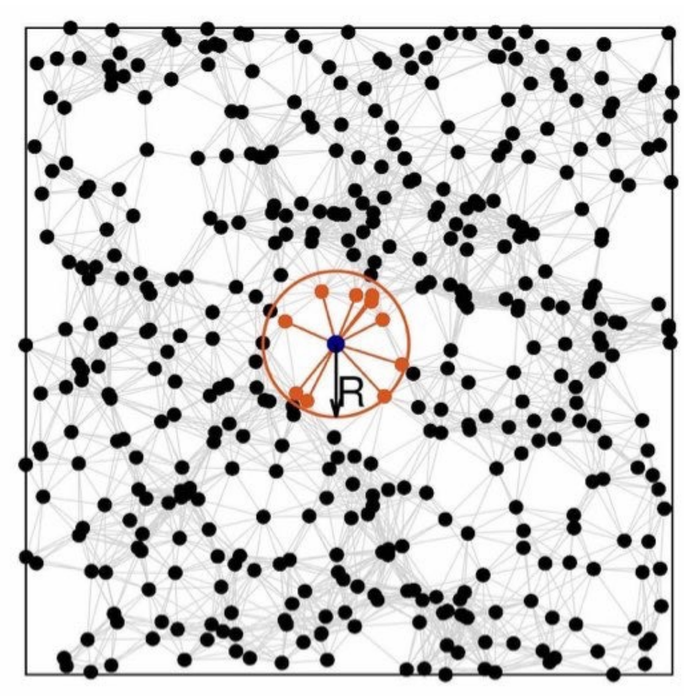
for instance: $$C_1 \equiv \frac{1}{2\pi} \int_{\mathbb{T}^2} f \in \mathbb{Z}.$$

integral over BZ

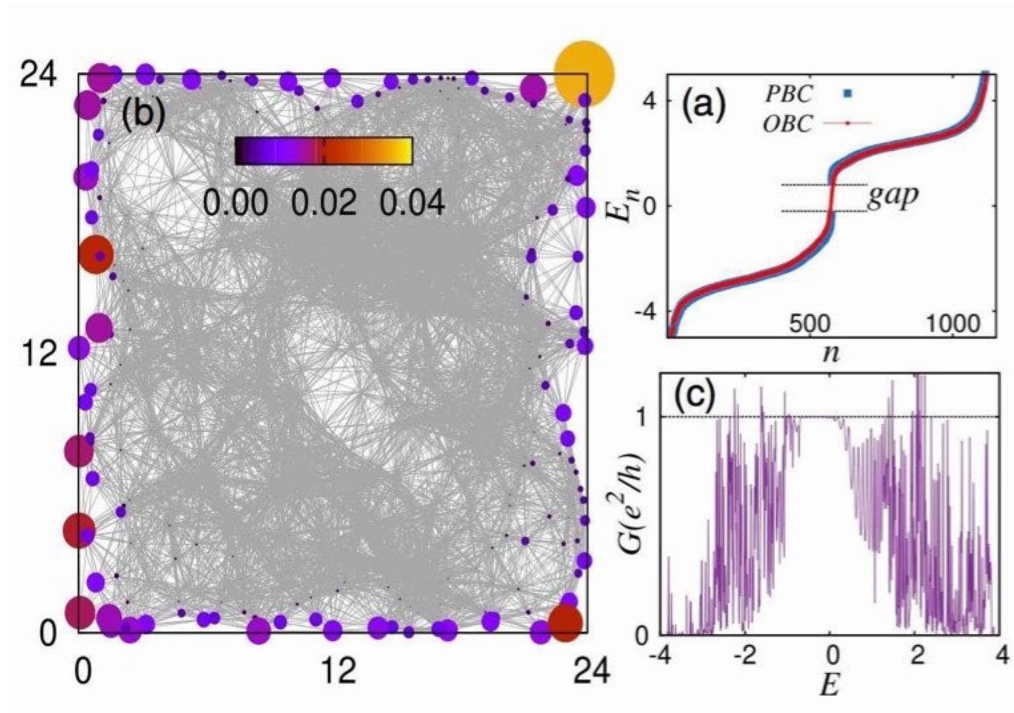


Amorphous topological insulators

Agarwala, Shenoy, PRL (2017)



random lattice



localized midgap states

$$\mathcal{H} = \sum_{I\alpha} \sum_{J\beta} t_{\alpha\beta}(\boldsymbol{r}_{IJ}) c^{\dagger}_{I,\alpha} c_{J,\beta}$$

Haldane + hopping

what is the topological invariant?

What about realistic systems?

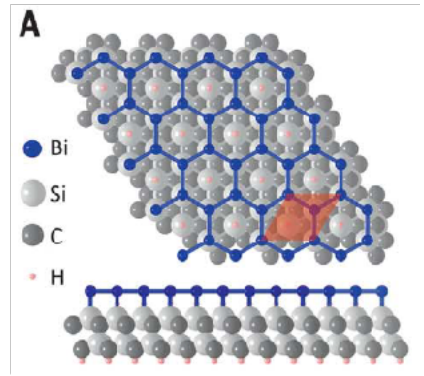
2D with strong SOC: bismuthene

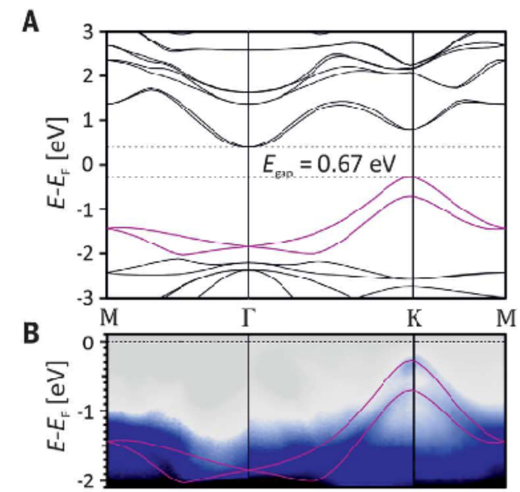
TOPOLOGICAL MATTER

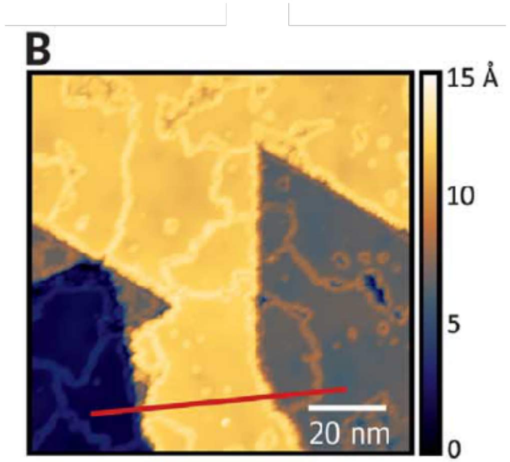
Bismuthene on a SiC substrate: A candidate for a high-temperature quantum spin Hall material

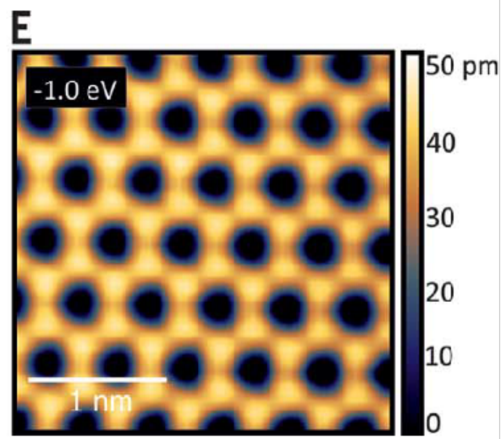
F. Reis,[1*] G. Li,[2,3*] L. Dudy,[1] M. Bauernfeind,[1] S. Glass,[1] W. Hanke,[3] R. Thomale,[3] J. Schäfer,[1†] R. Claessen[1]

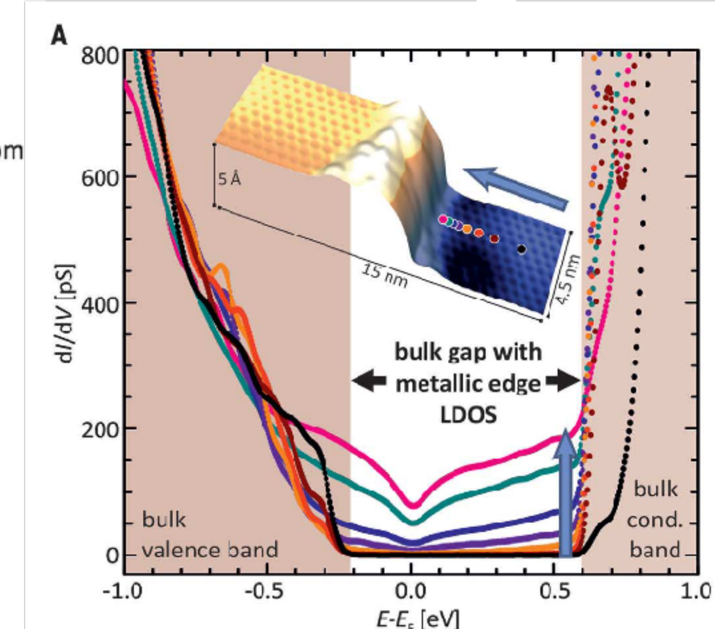
Science (2017)



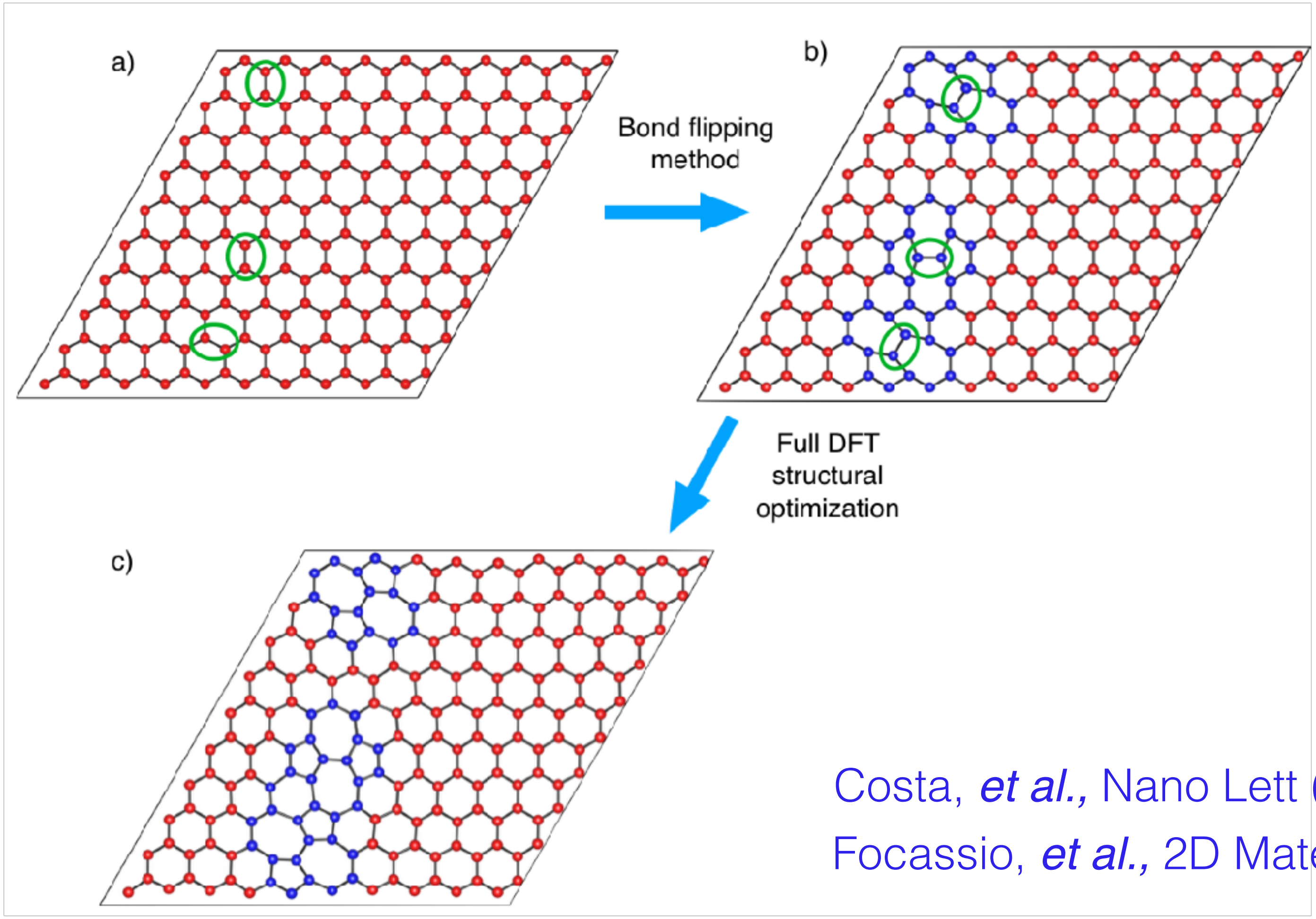








"Amorphization" route



Costa, *et al.*, Nano Lett (2019)

Focassio, *et al.*, 2D Mater (2021)

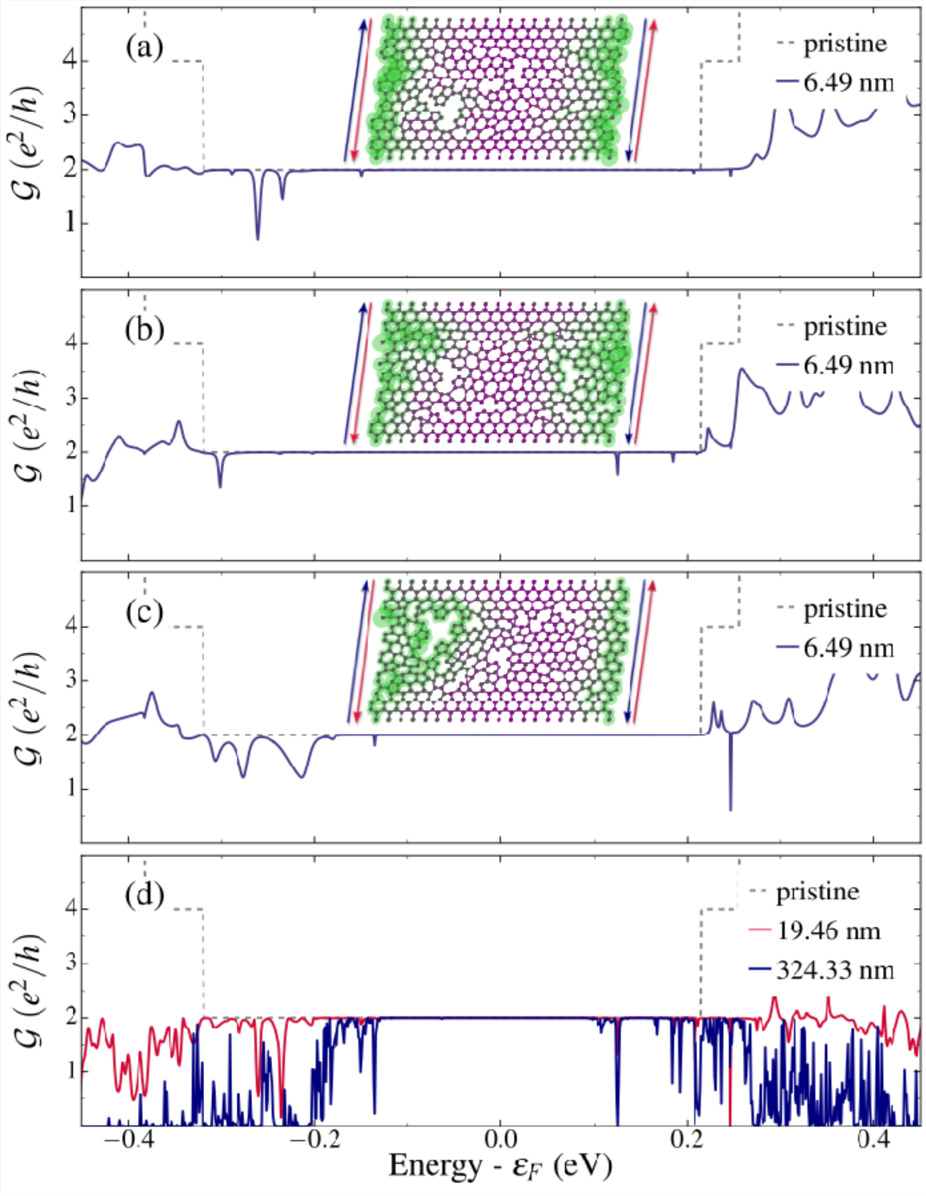
Realistic amorphous topological insulators

linear conductance

$$\mathcal{G} = \frac{e^2}{h} \int \mathcal{T}(E) \left(-\frac{\partial f}{\partial E} \right) \mathrm{d}E$$

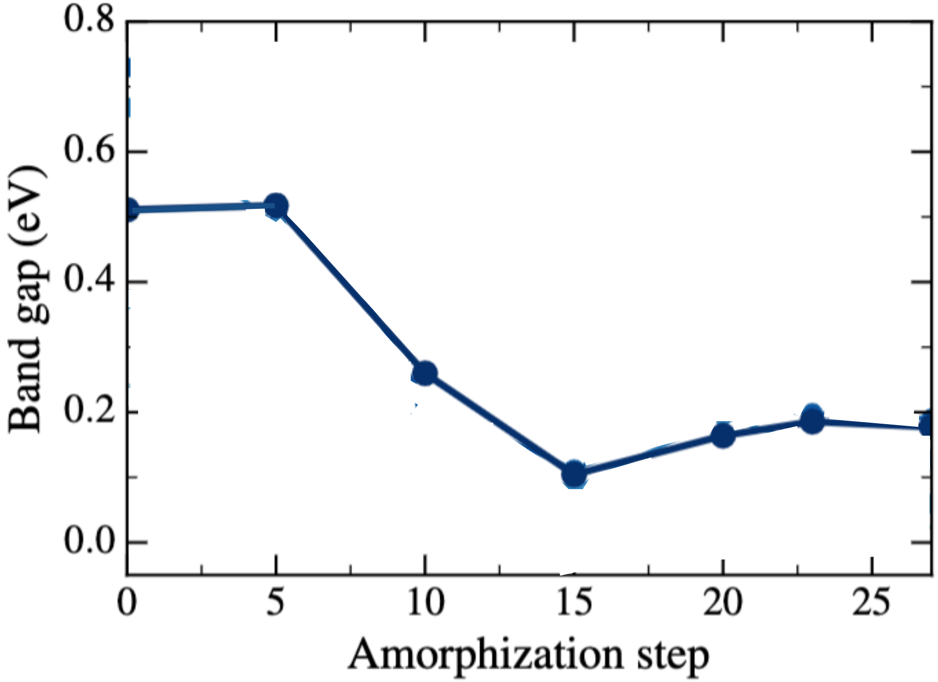
transmission

$$\mathcal{T}(E) = \mathrm{Tr}[\mathbf{\Gamma}_L \mathbf{G}_S \mathbf{\Gamma}_R \mathbf{G}_S^{\dagger}]$$

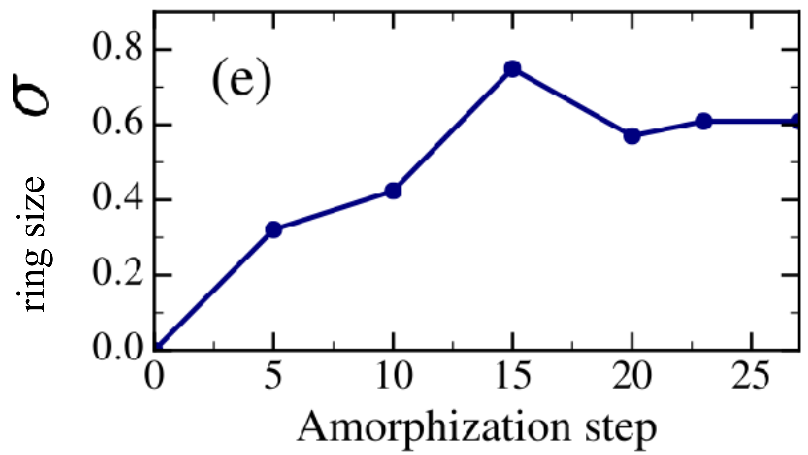


"Very” amorphous?

energy band gap

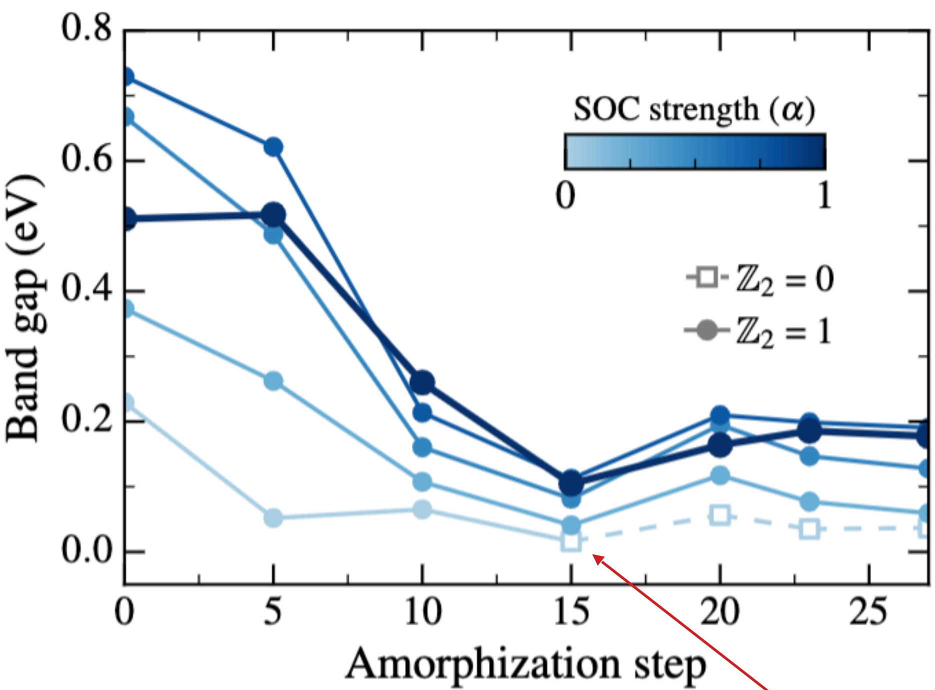


ring size variance

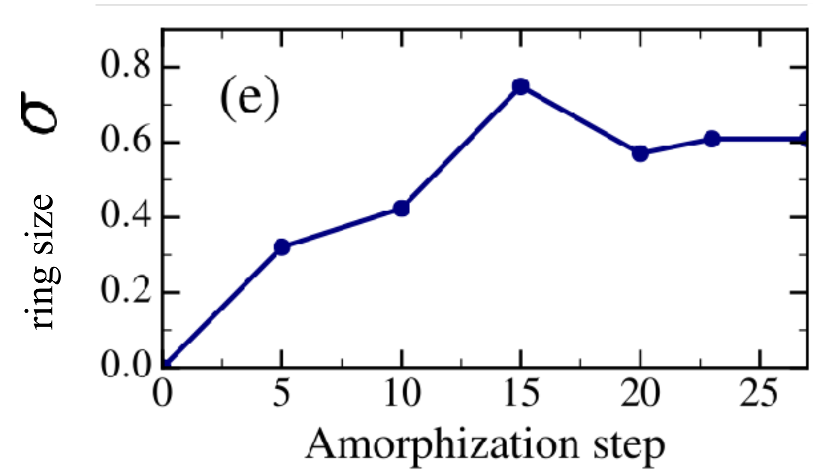


"Very" amorphous?

energy band gap



ring size variance



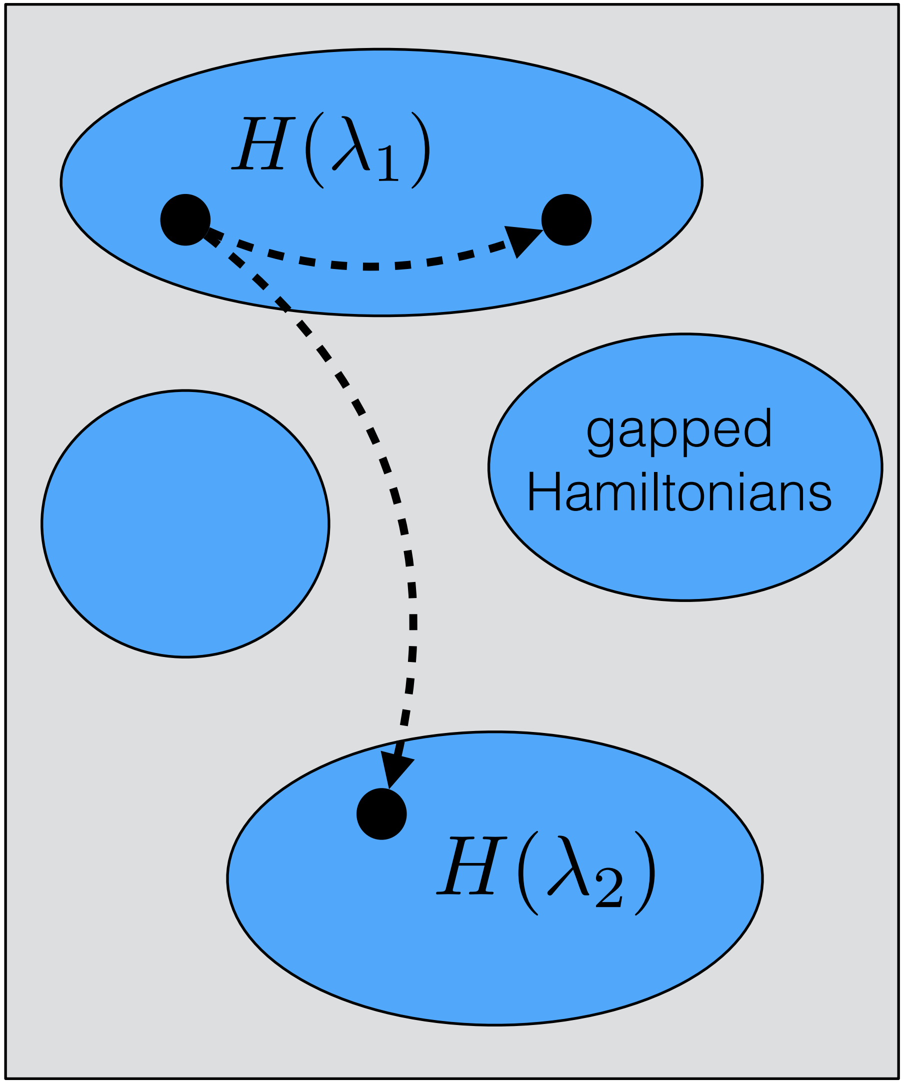
phase transition

Topological Phase Transitions

Schematic picture

Definition:

Two states are in the same topological phase if they can be *smoothly* transformed into each other without closing the gap

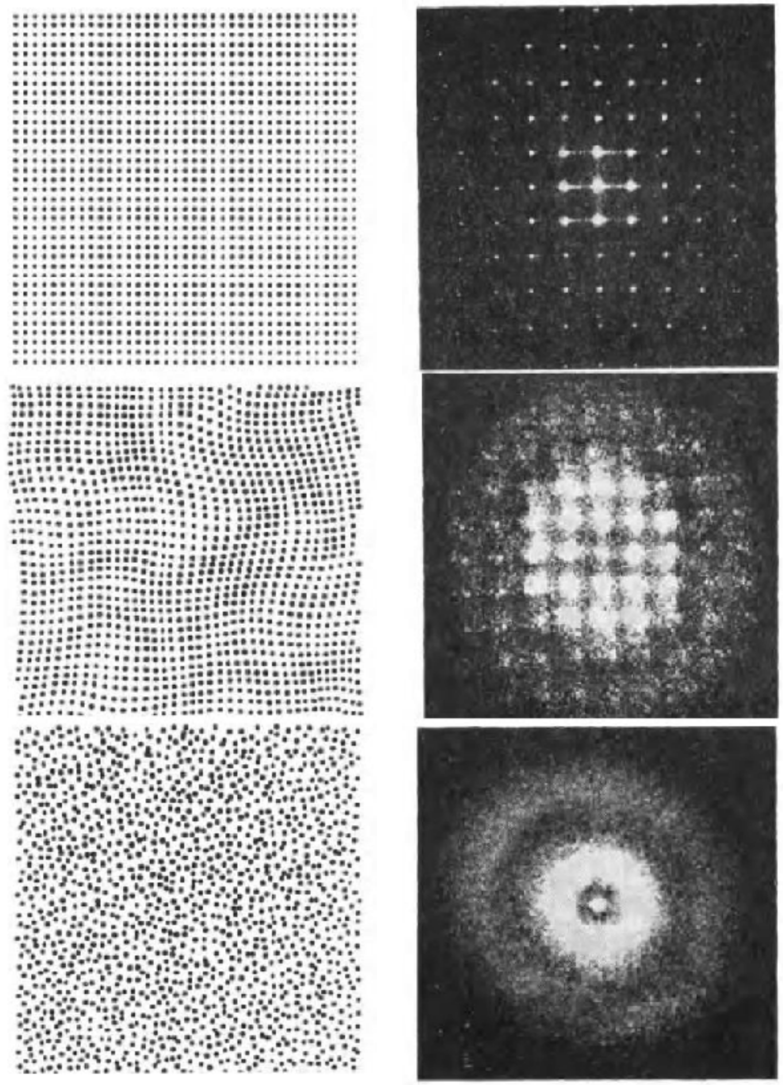


Transition: Paracrystals

Victor Regis
(Ljubliana)

Marcello Silva Neto
(UFRJ)

lattice structure   diffraction pattern



Hosemann paracrystals:
medium range order

Disorder model:
Perlin noise

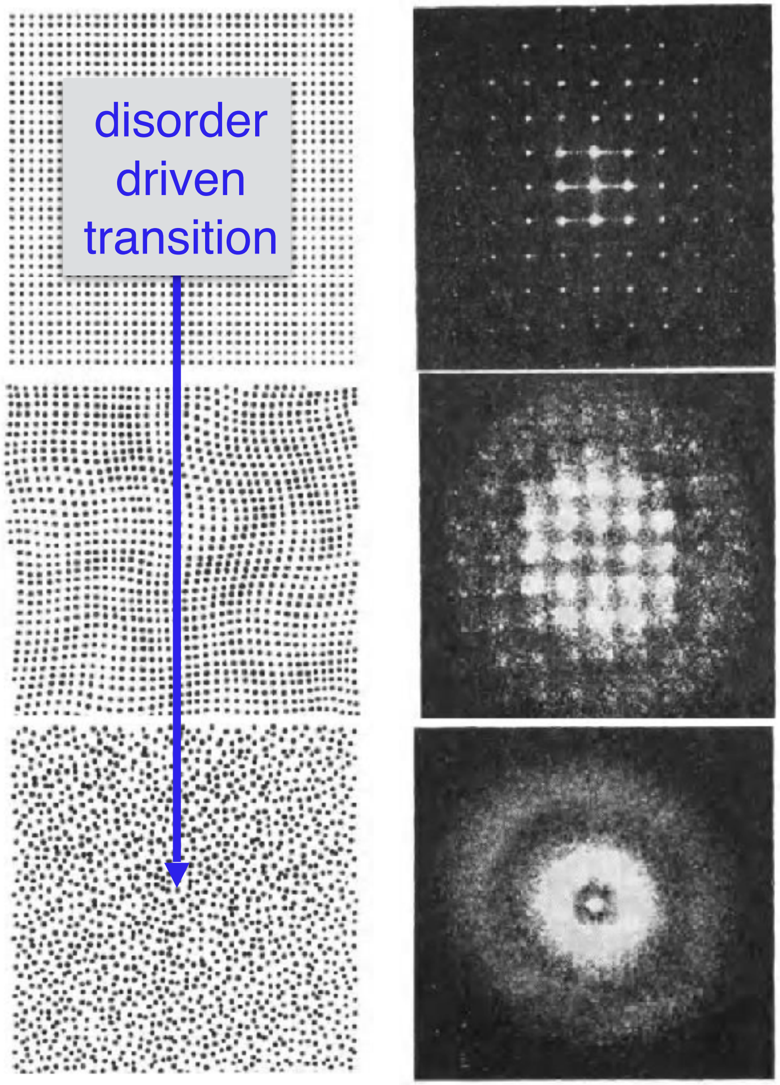
amorphous phase

Transition: Paracrystals

Victor Regis
(Ljubliana)

Marcello Silva Neto
(UFRJ)

lattice structure | diffraction pattern



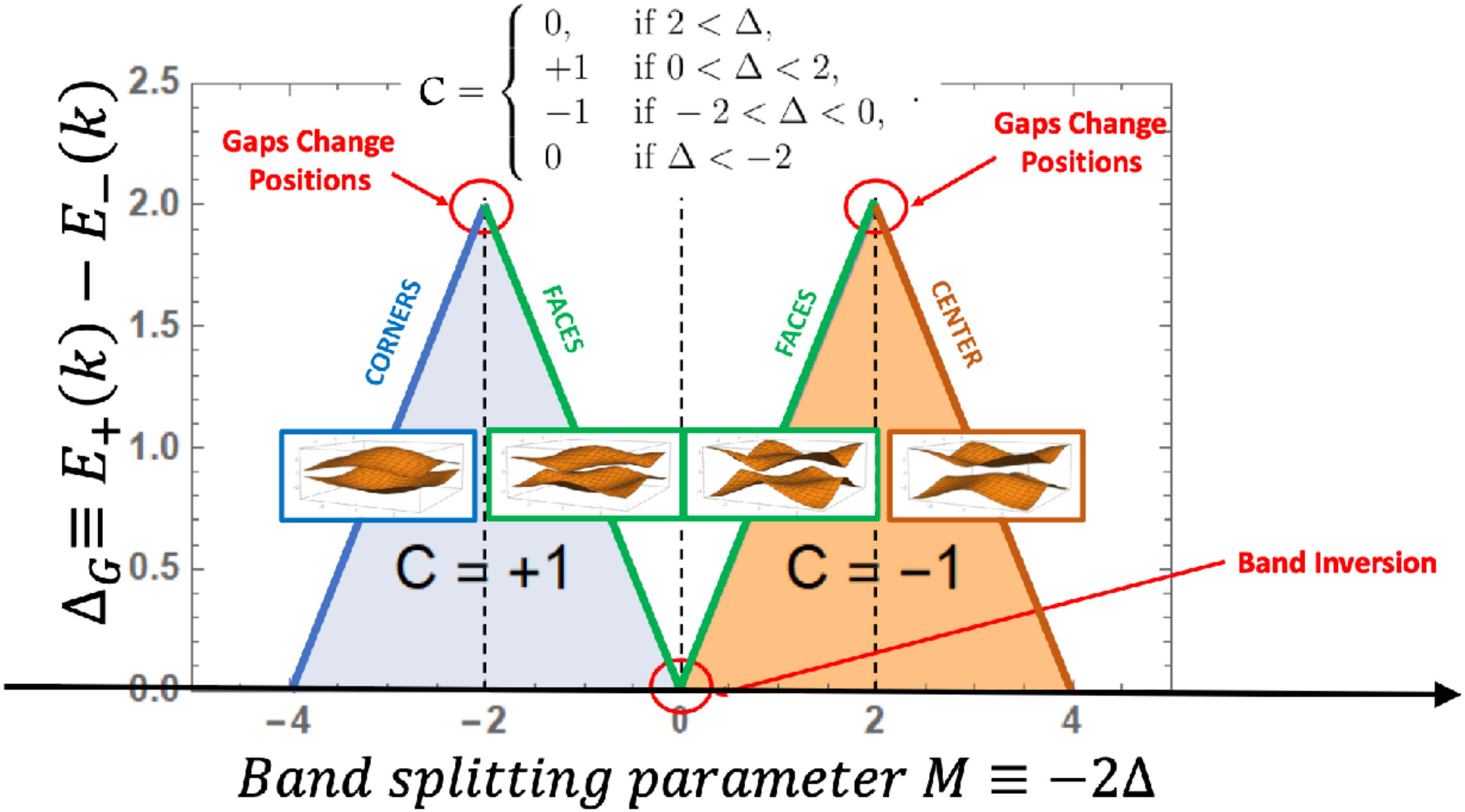
Hosemann paracrystals:
medium range order

amorphous phase

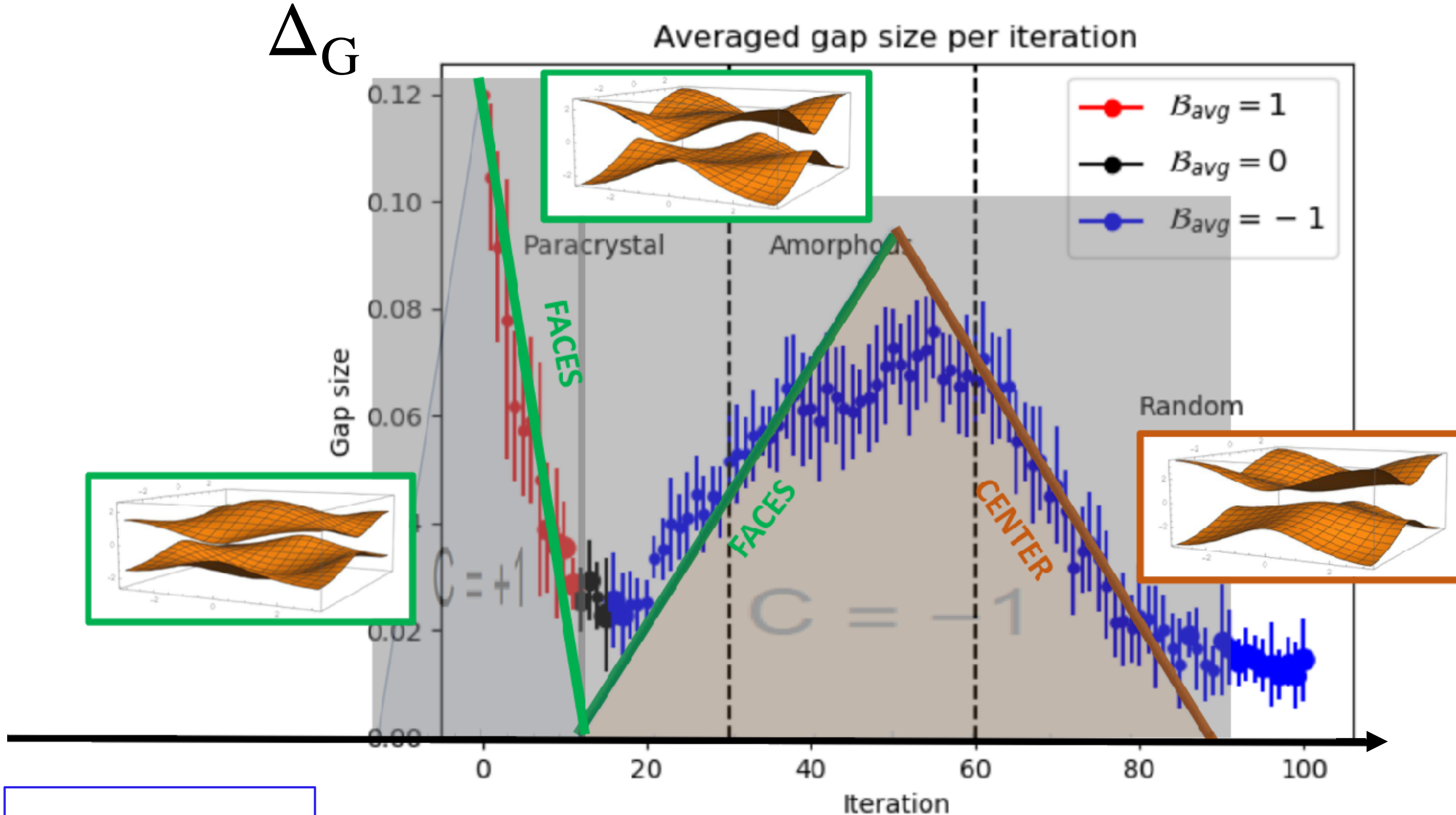
Disorder model:
Perlin noise

Structurally driven topological phase transition

Topological phase diagram - half-BHZ model



Structurally driven topological phase transition



$Re[\Sigma(\mathbf{k}, \lambda)]$

amorphization

Local topological invariants

- Chern number in real space

Bianco & Resta, PRB(R) (2011)

$$\mathcal{C} = -\frac{1}{\pi}\mathrm{Im}\sum_{n=1}^{N_c}\int_{\mathrm{BZ}} d\mathbf{k}\left\langle \frac{\partial}{\partial k_x}u_{n\mathbf{k}}\middle| \frac{\partial}{\partial k_y}u_{n\mathbf{k}}\right\rangle$$

standard expression

$$\mathcal{C} = -2\pi i\,\mathrm{tr}\{[PxP, PyP]\}$$

$$P = \sum_{n=1}^{N_c}\int \frac{d\mathbf{k}}{(2\pi)^2}|\psi_{n\mathbf{k}}\rangle\langle\psi_{n\mathbf{k}}|$$

- Local markers

projectors: $$X(\mathbf{r},\mathbf{r}') = \int d\mathbf{r}'' P(\mathbf{r},\mathbf{r}'')x'' P(\mathbf{r}'',\mathbf{r}')$$

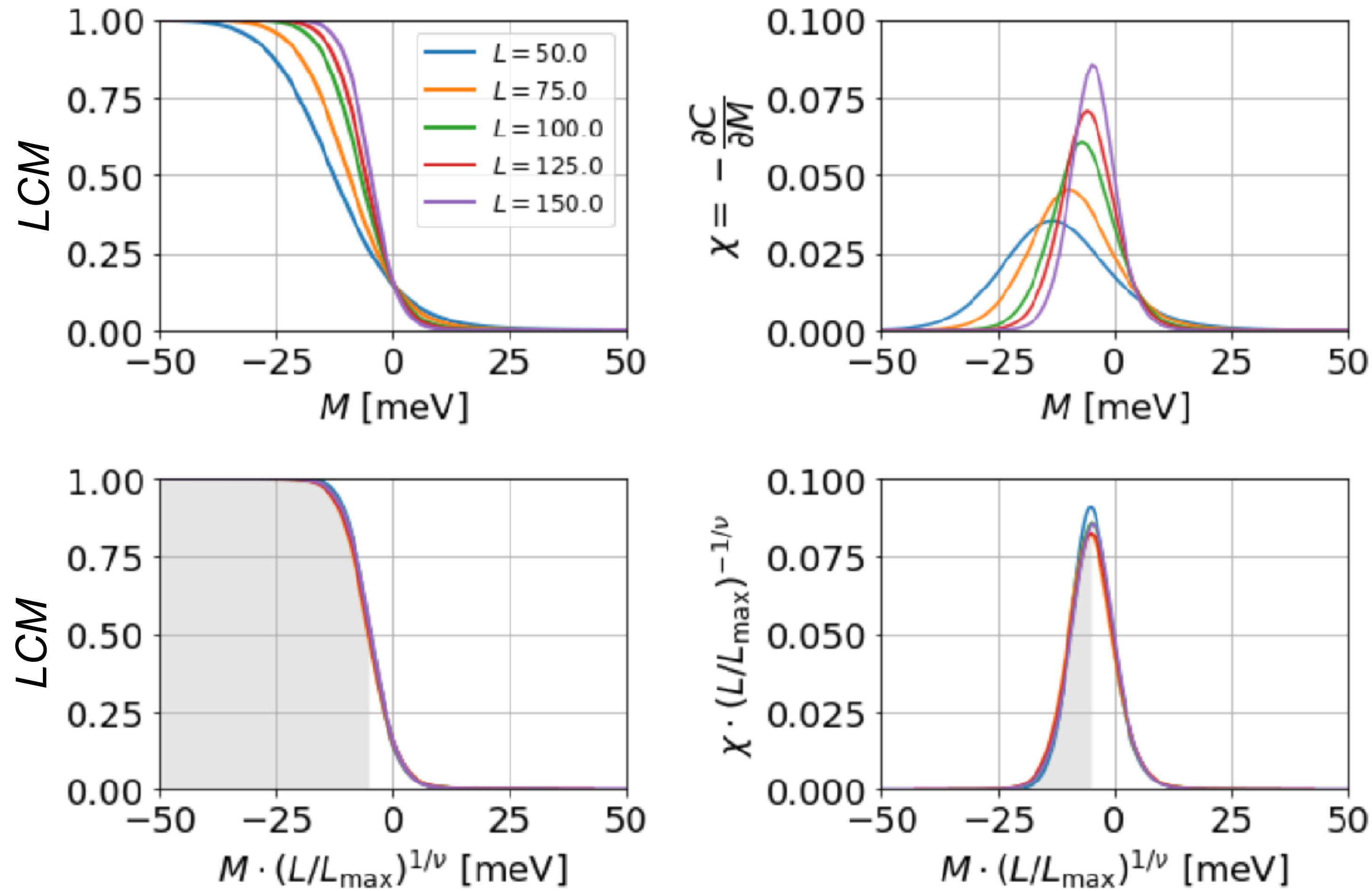
$$\mathcal{C}(\mathbf{r}) = -2\pi i\int d\mathbf{r}'\left[X(\mathbf{r},\mathbf{r}')Y(\mathbf{r}',\mathbf{r}) - Y(\mathbf{r},\mathbf{r}')X(\mathbf{r}',\mathbf{r})\right]$$

Song and Prodan, PRB (2014)
Mondragon-Shem, *et al.*, PRL (2015)
Varjas, *et al.*, PRR (2020), Chen, *et al*, arXiv (2022)

Pristine BHZ: topological phase transition

mass driven phase transition

critical exponent $\nu = 1.16$



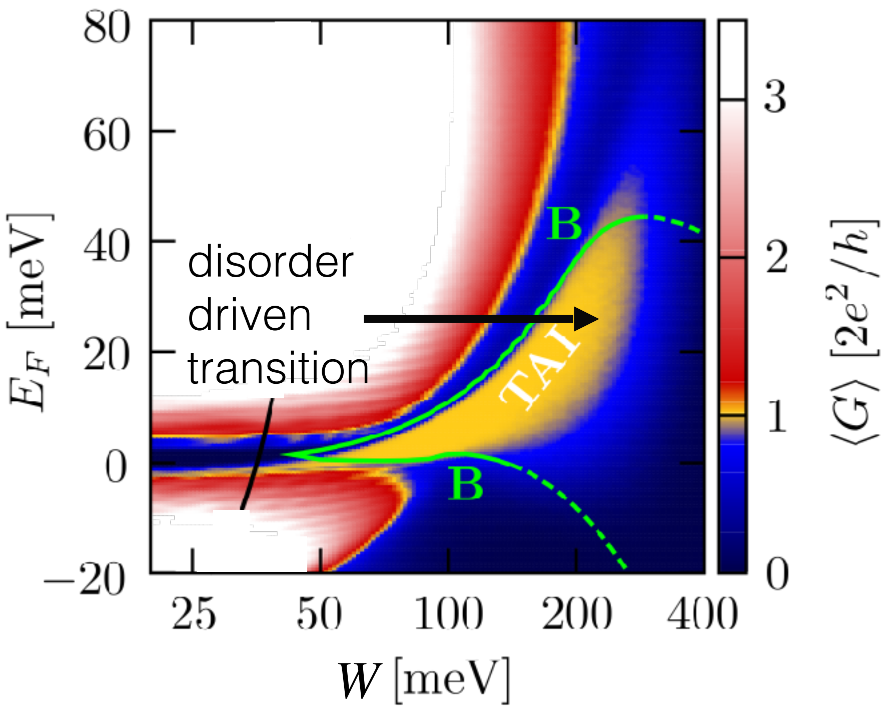
Kane Mele model: Caio, *et al.* Nat. Phys (2017)

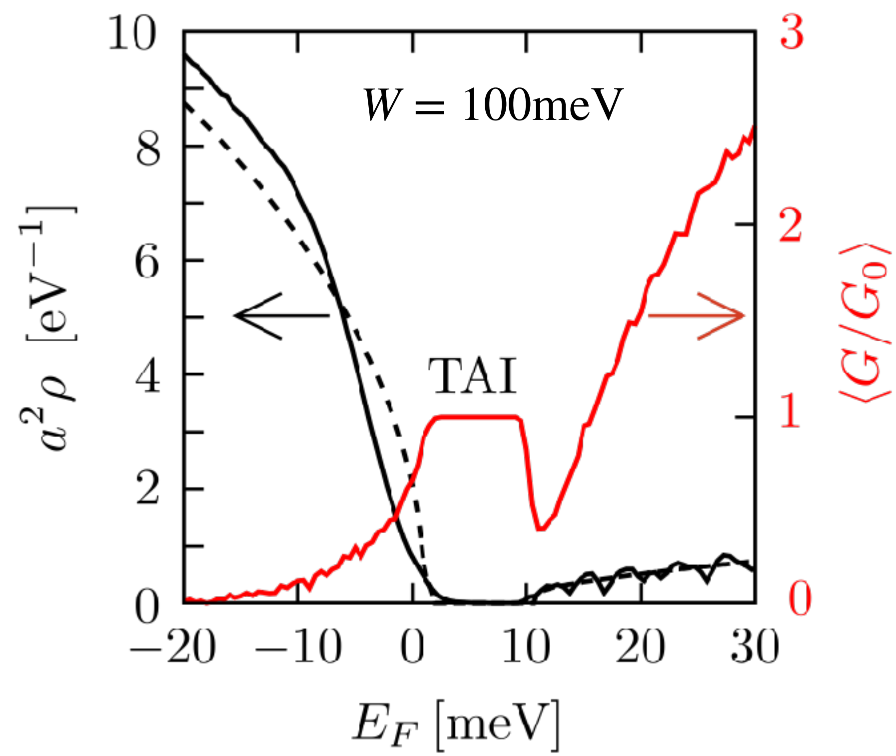
Wei Chen *et al*, momentum space

Anderson topological insulators

BHZ model $H = \alpha(p_x\sigma_x - p_y\sigma_y) + (m + \beta p^2)\sigma_z + [\gamma p^2 + U(\mathbf{r})]\sigma_0.$

Anderson disorder





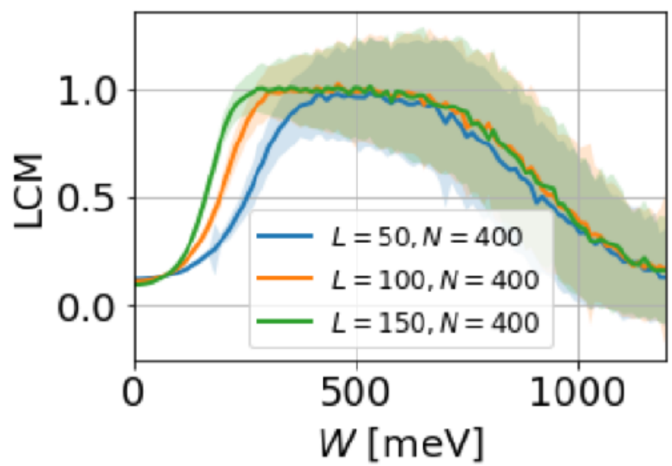
Li, et al. PRL (2009)

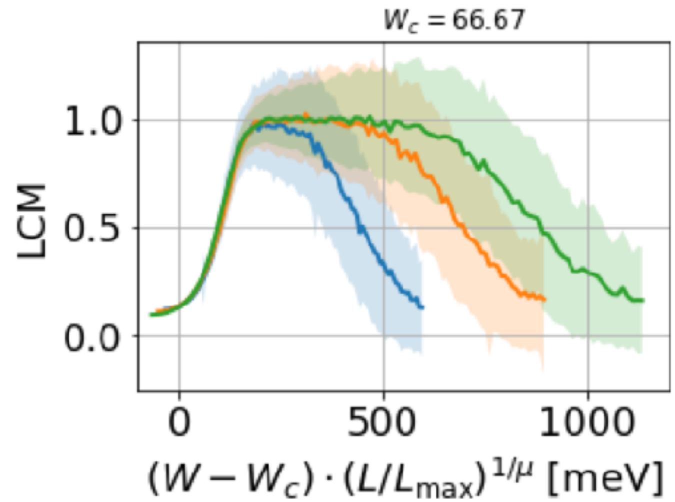
Groth, et al. PRL (2009)

Disordered BHZ: topological phase transition

disorder driven phase transition

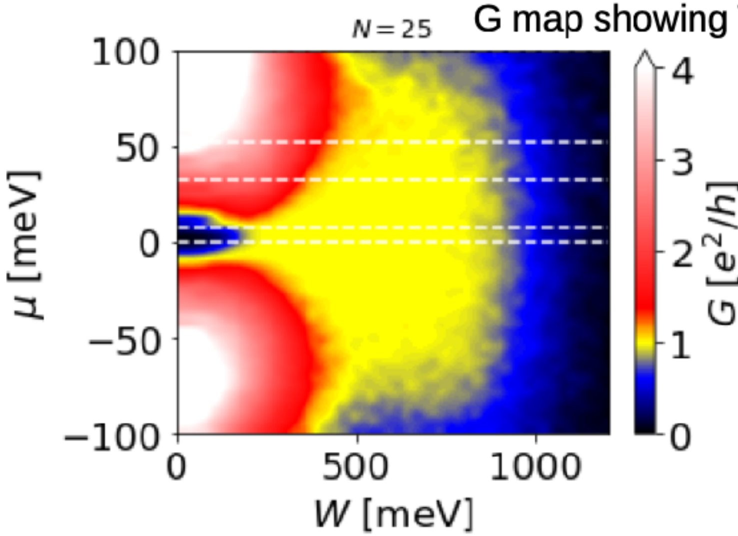
with B. Assunção and Gerson Ferreira

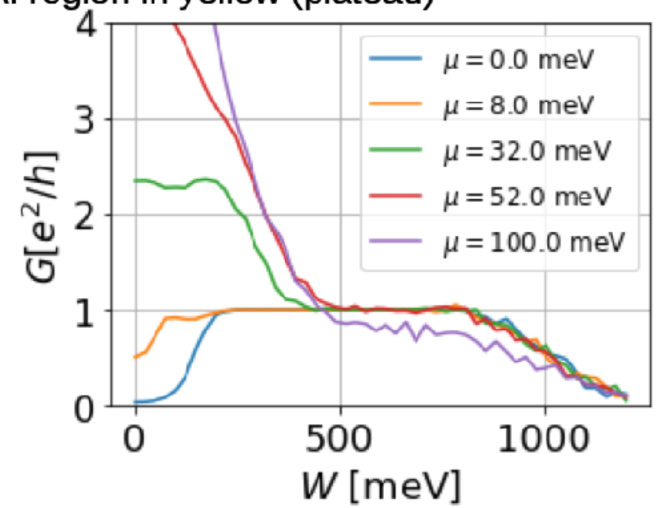




$\mu = 2$

G map showing TAI region in yellow (plateau)

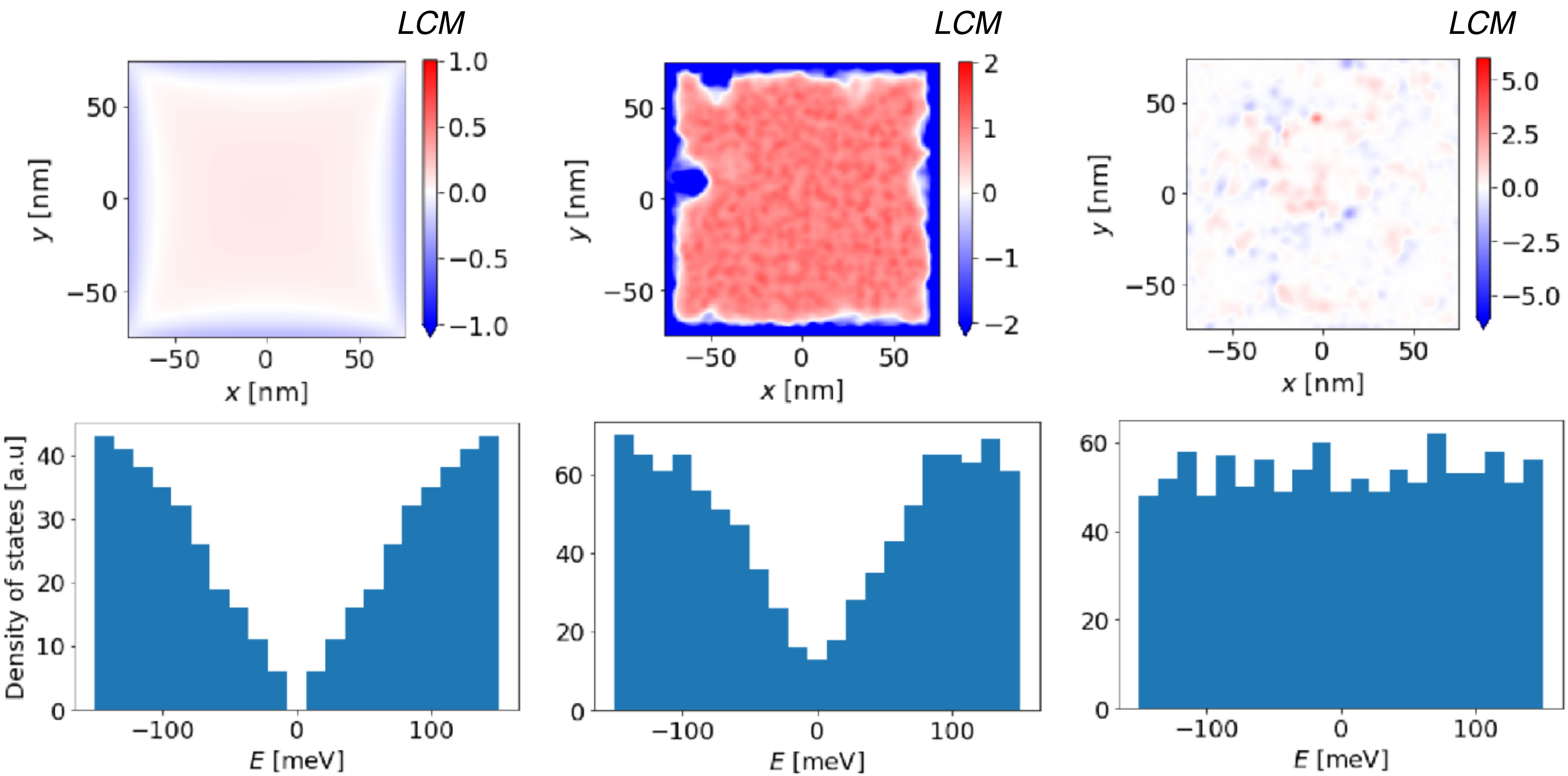




Local Chern marker: different disorder strengths

single realization: $M = 2$ meV, $L = 150$ nm

LCM at $E_F = 0$



clean system | $W = 500\text{meV}$ | $W = 1200\text{meV}$

Summary

- Theory of topological insulators is based on band structure properties
- For strongly disordered systems the transport properties have only a weak relation with the pristine material electronic structure.
- Yet: strongly disordered systems show topological properties.
- Challenges:
  How to describe metal-insulator transitions (closing of the topological gap) in such systems?
  Quest for a *bona fide* real space topological invariant

Mathematics: Rigorous real space invariant

K-theory:

construction of families of K-functions that map topological spaces into a much simpler ring structure.

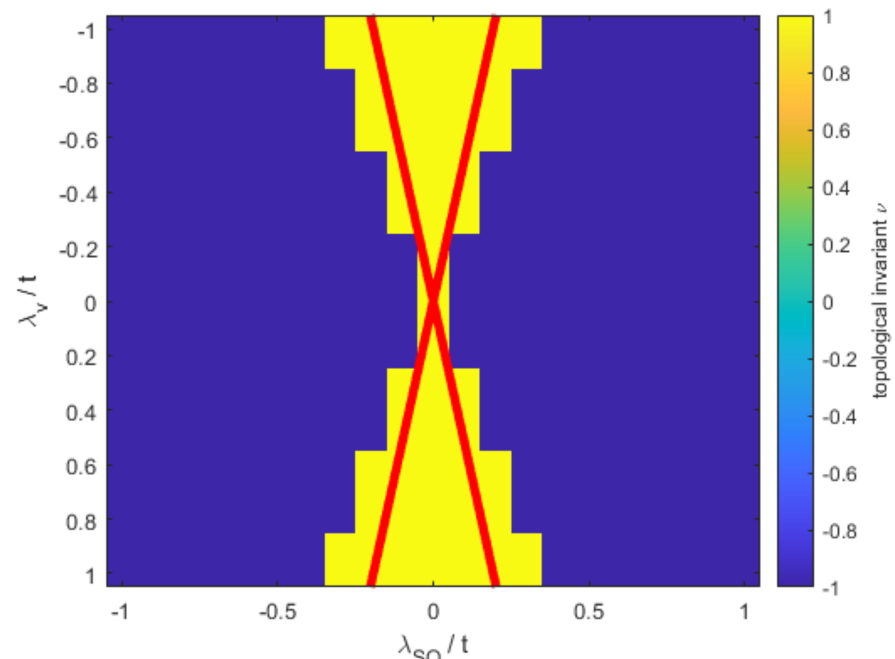
functional mapping makes easier to compute topological properties

examples of applications: Bott periodicity, Atiyah-Singer index theorem

Roe-C* algebras

The K-Theory of $C^*_{\text{Roe}}(R^d)$ with symmetries reproduces the Altland-Zirnbauer classes.

Phase diagram of Kane-Mele model



collaboration
Regensburg (Math)
Christoph Setescak,
Mathias Ludewig

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Collaborators

Adalberto Fazzio (CNPEM, Brazil), Bryan Assunção (UFU, Brazil), Bruno Focassio (UFABC), Chris Setescak (Regensburg, Germany), Felipe Lima (CNPEM, Brazil), Gabriel Schleder (CNPEM, Brazil), Gerson Ferreira (UFU, Brazil), Marcelo Silva Neto (UFRJ, Brazil), Marcio Costa (UFF, Brazil), Mathias Ludewig (Regensburg, Germany), Victor Regis (Liubliana, Eslovênia)

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CNPq
Conselho Nacional de Desenvolvimento Científico e Tecnológico

CAPES

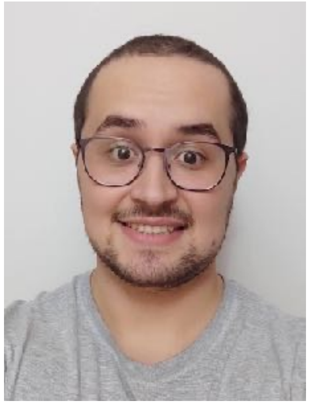
Search for 3D amorphous TIs

Experiments:
$Bi_{1-x}Sb_x$ alloys,
"pristine" layered chalcogenides
(Bi_2Se_3, Bi_2Te_3, Sb_2Te_3)

Experiments:
amorphous Bi_2Se_3
Nature Mater. **22**, 200 (2023)

Amorphous Bi_2Se_3 structural, electronic, and topological nature from first principles

PRB (2021)

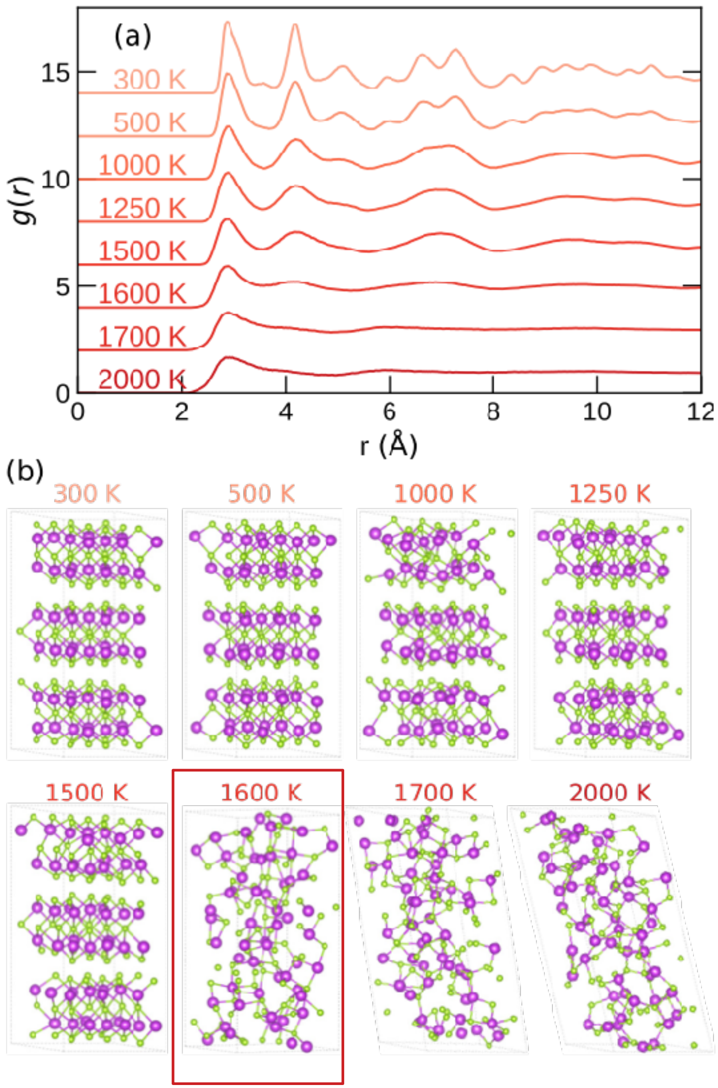

Bruno Focassio (UFABC)


Felipe Lima (CNPEM)


Gabriel Schleder (Harvard)


Adalberto Fazzio (CNPEM)

Structural properties



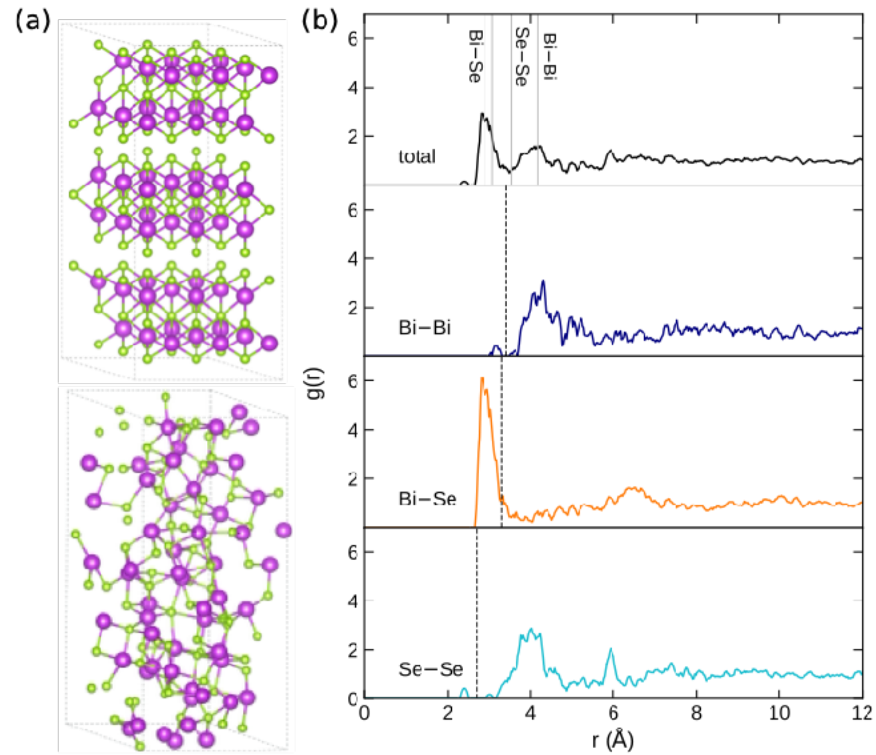
transition

simulated annealing

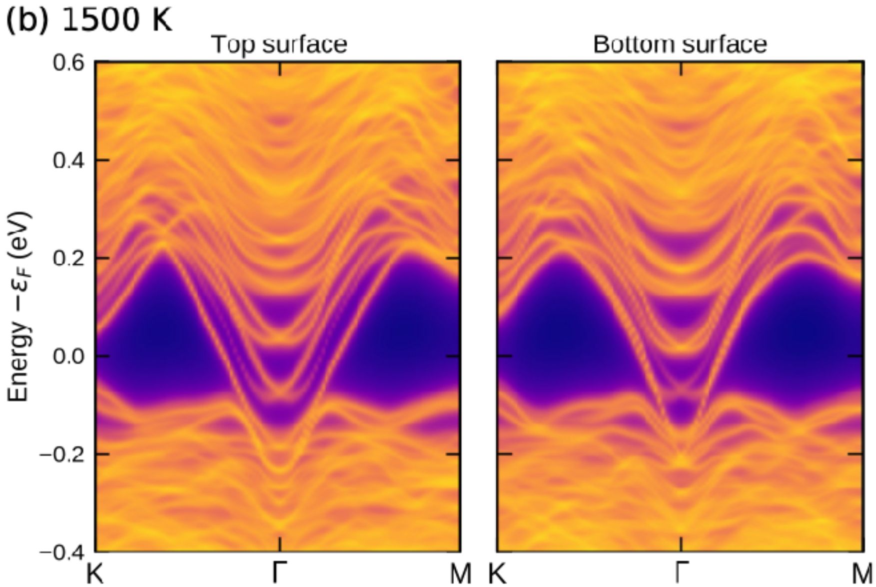
NVT, 10ps annealing steps

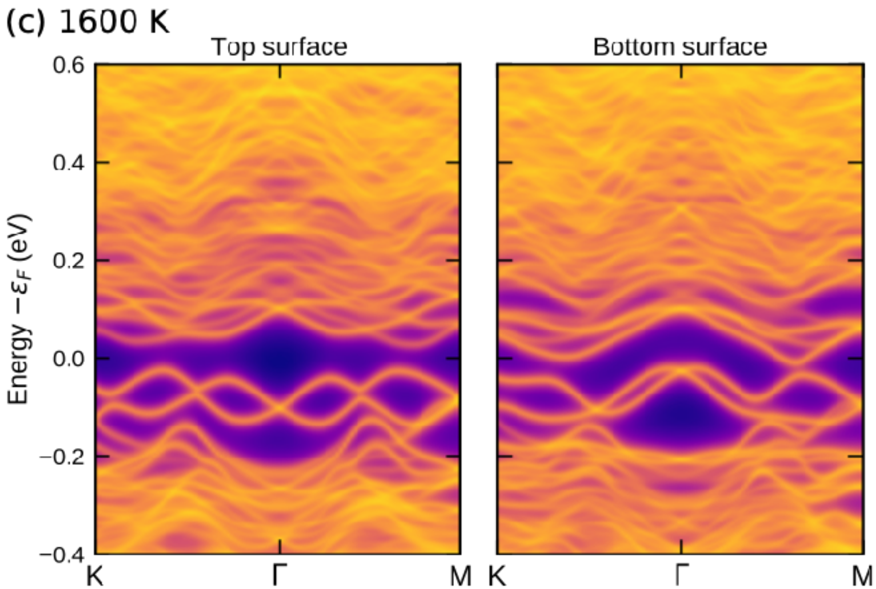
pristine vs. amorphous

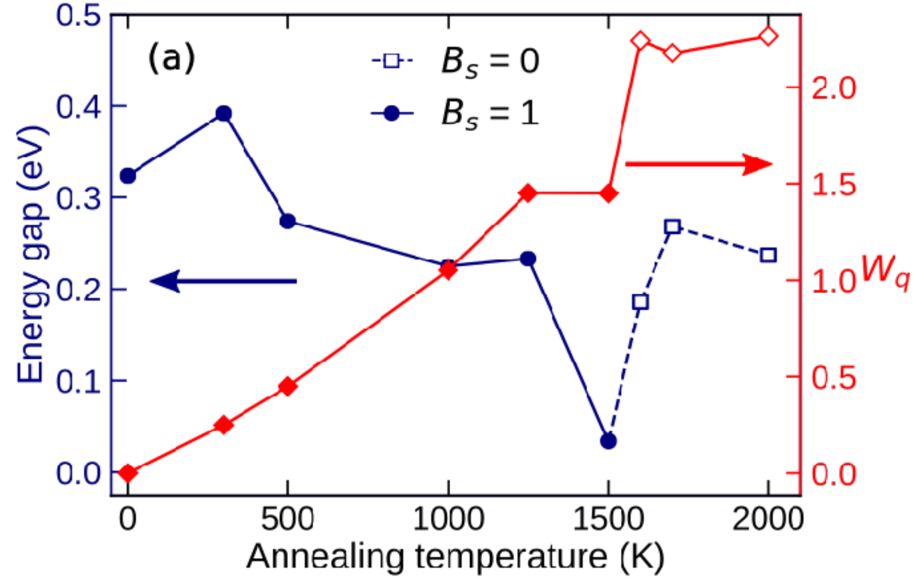
lack of octahedral coordination



Electronic properties







local order parameter

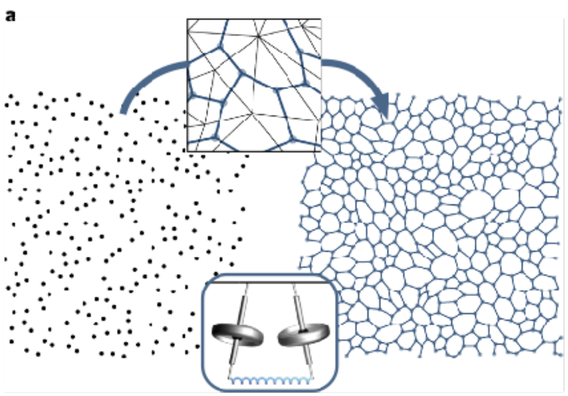
$$q_j = 1 - \frac{3}{8}\sum_{i>k}\left(\frac{1}{3} + \cos\theta_{ijk}\right)^2$$

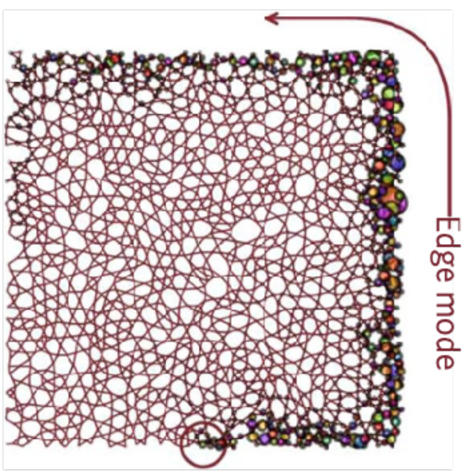
$$W_q = \left\langle q_j \right\rangle$$

Amorphous topological insulators: experiments

Mitchel et al., Nat. Phys. (2018)

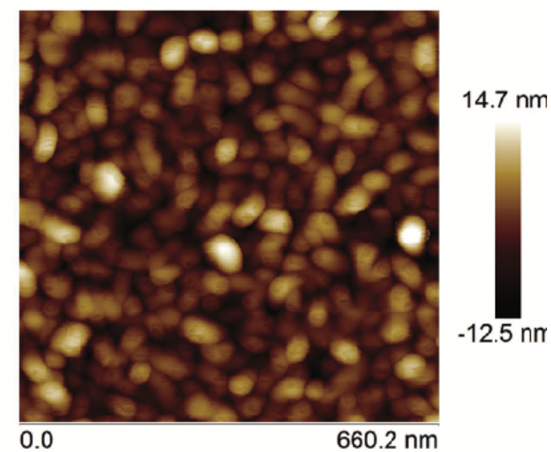
metamaterial - "gyroscopes"

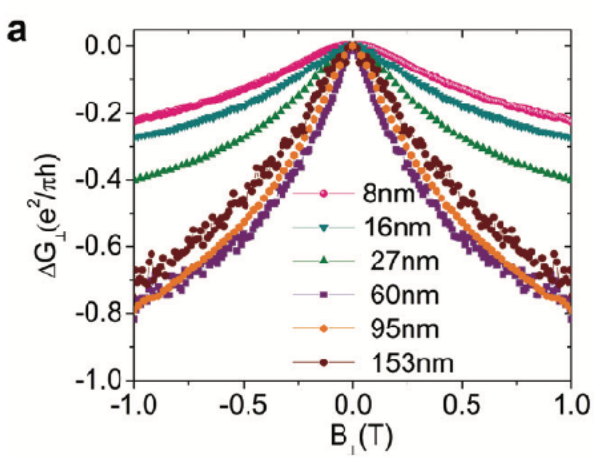




Banerjee et al., Nanoscale (2017)

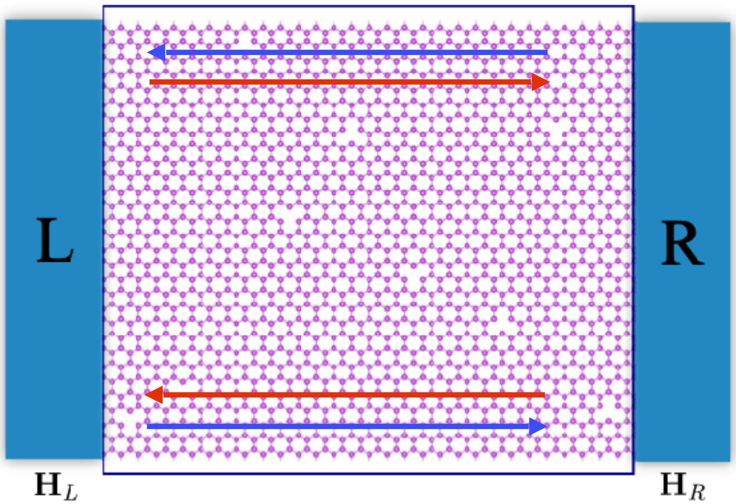
granular films of Bi_2Se_3

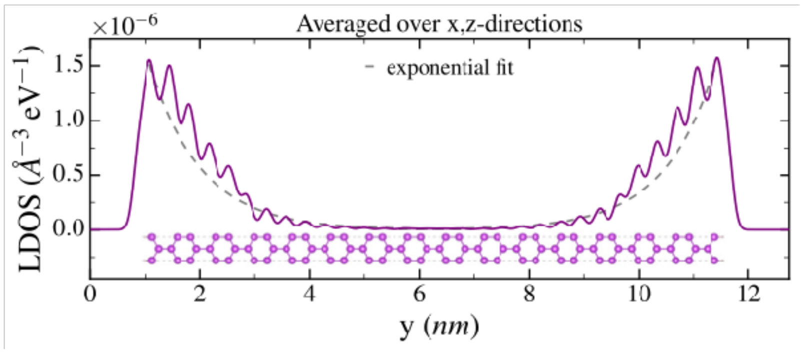


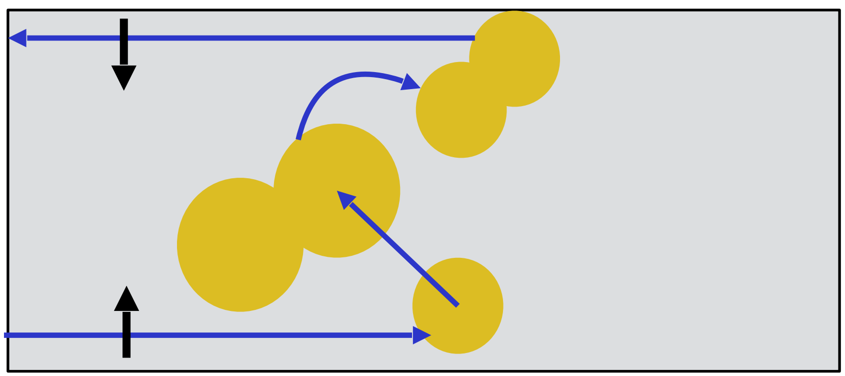


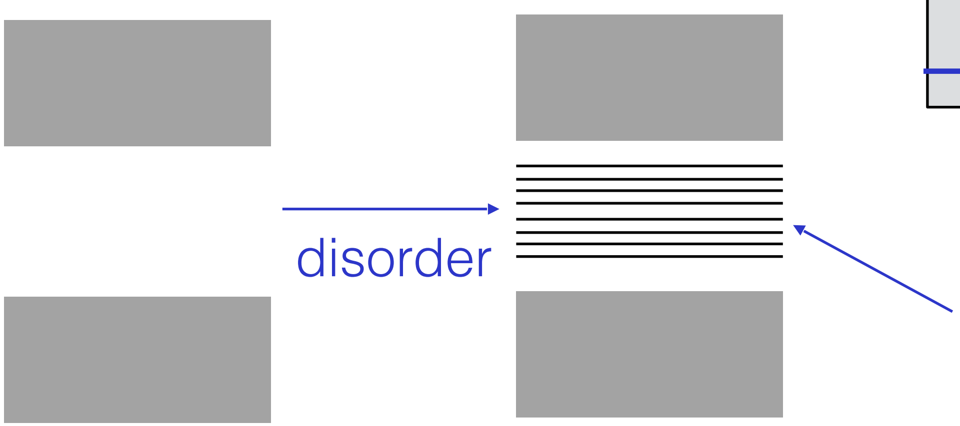
Disorder and transport

Pezo *et al.*, PR Materials (2021): vacancies in bismuthene









localized states

long range hopping?

Voronoi lattices

RESEARCH ARTICLE

Topological Weaire–Thorpe models of amorphous matter

Quentin Marsal, Dániel Varjas, and Adolfo G. Grushin

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