

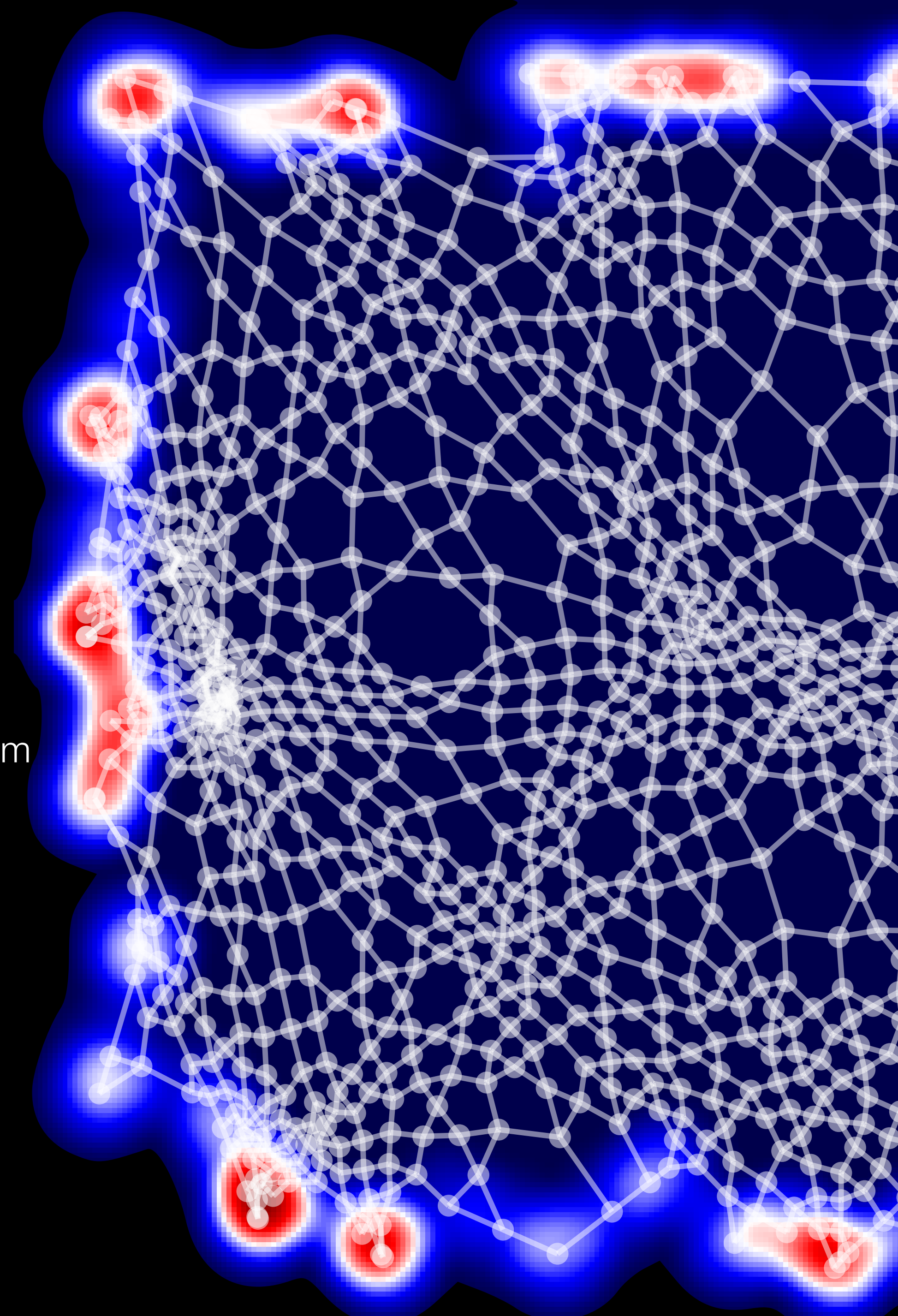
# Amorphous topological solids

from flat bands to chiral spin liquids

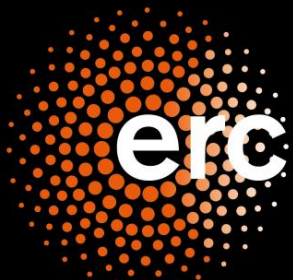
Adolfo G. Grushin, Néel Institute, CNRS

KITP— March 30th, 2023

A Quantum Universe in a crystal: Symmetry and Topology across the Correlation Spectrum

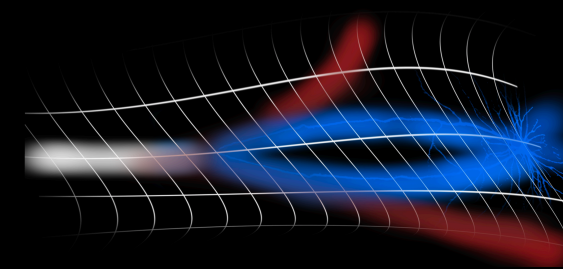


TOPOMORPH



European Research Council  
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FET-OPEN  
SCHINES



AGENCE NATIONALE DE LA RECHERCHE  
ANR

# Amorphous topological solids

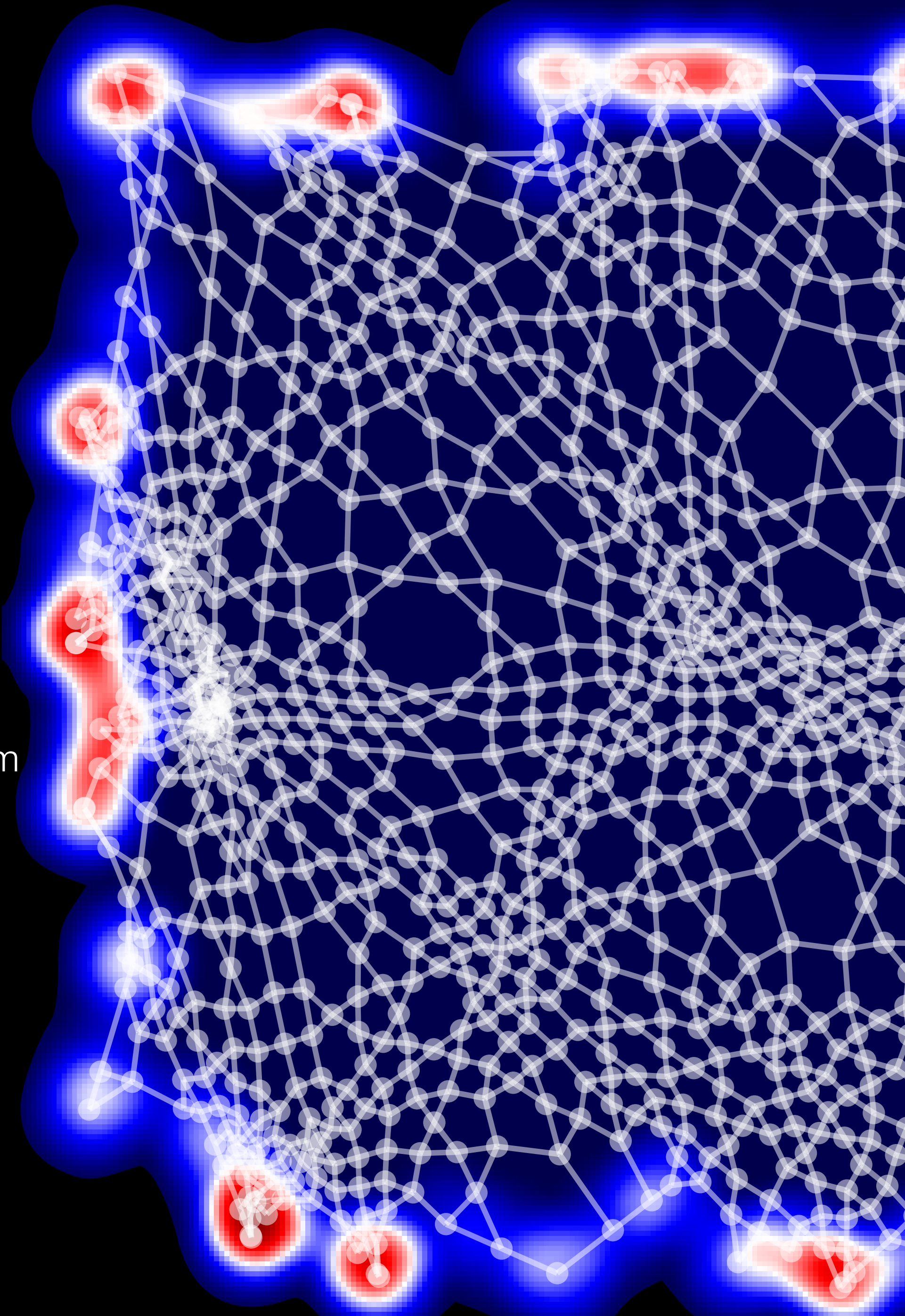
from flat bands to chiral spin liquids

Adolfo G. Grushin, Néel Institute, CNRS

KITP— March 30th, 2023

A Quantum Universe in a **crystal**: Symmetry and Topology across the Correlation Spectrum

**lattice**

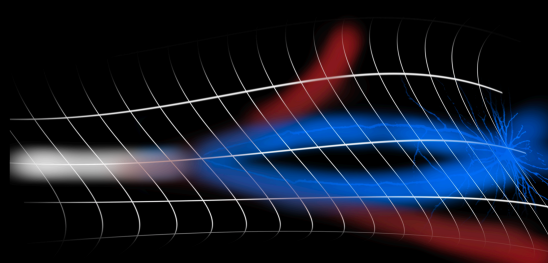


TOPOMORPH



European Research Council  
Established by the European Commission

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SCHINES

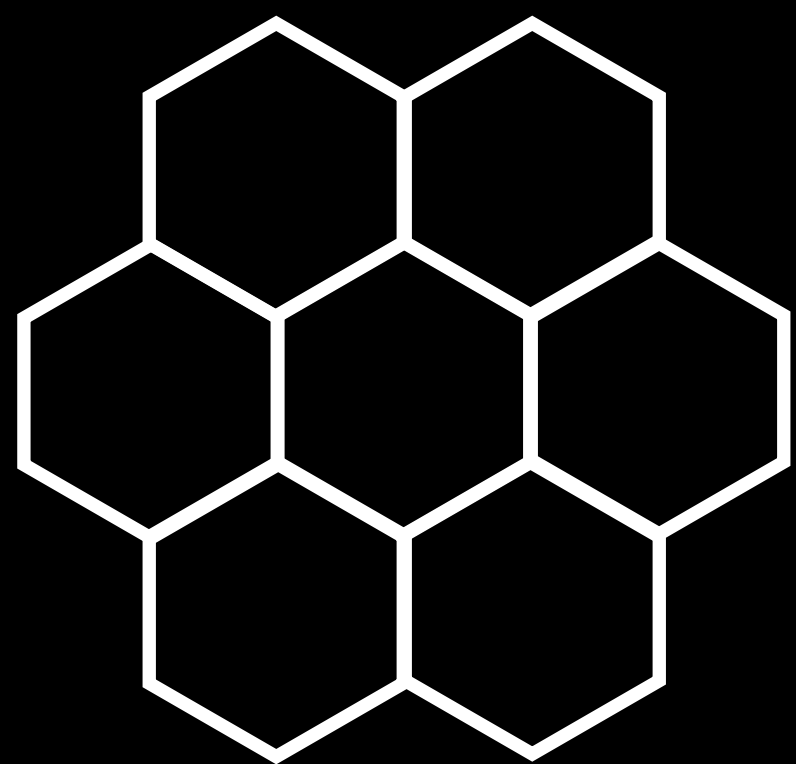


AGENCE NATIONALE DE LA RECHERCHE  
**ANR**



# How do we find new topological insulators?

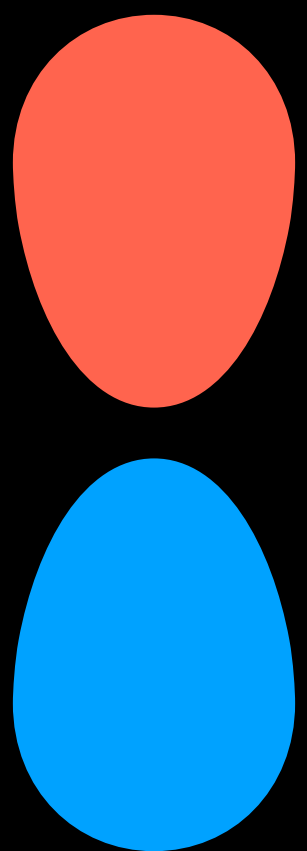
## Space Group



— lattice symmetries

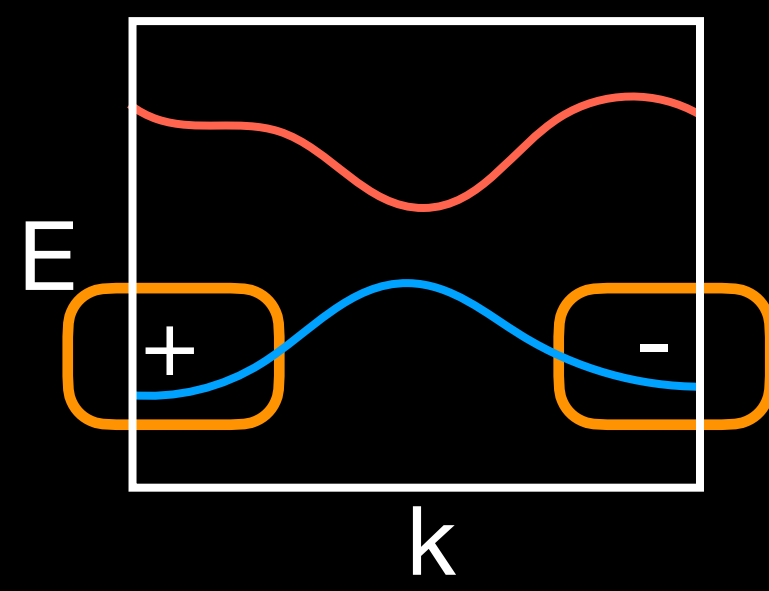
translations, rotations, inversions, mirrors

## Orbitals



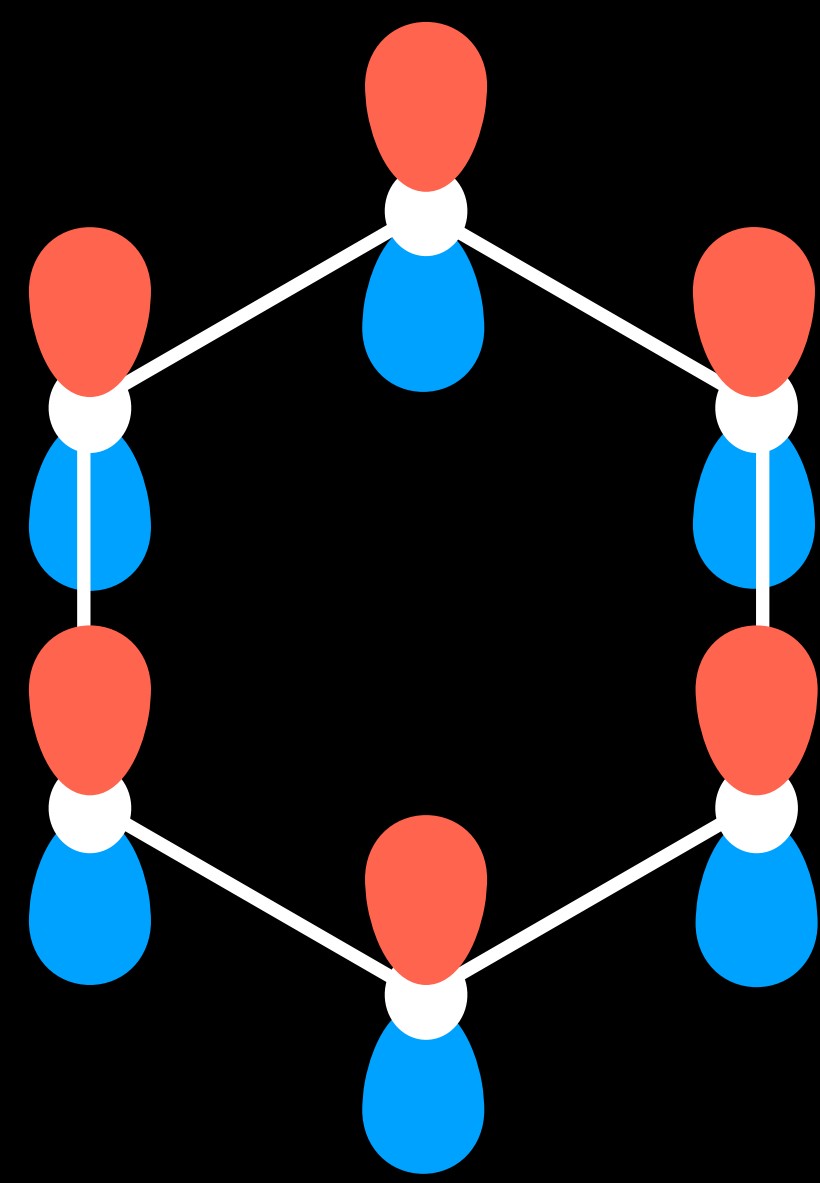
— wavefunctions

s, p, d...



— band connectivity + symmetries labels

## Atomic positions



# How do we find new topological insulators?

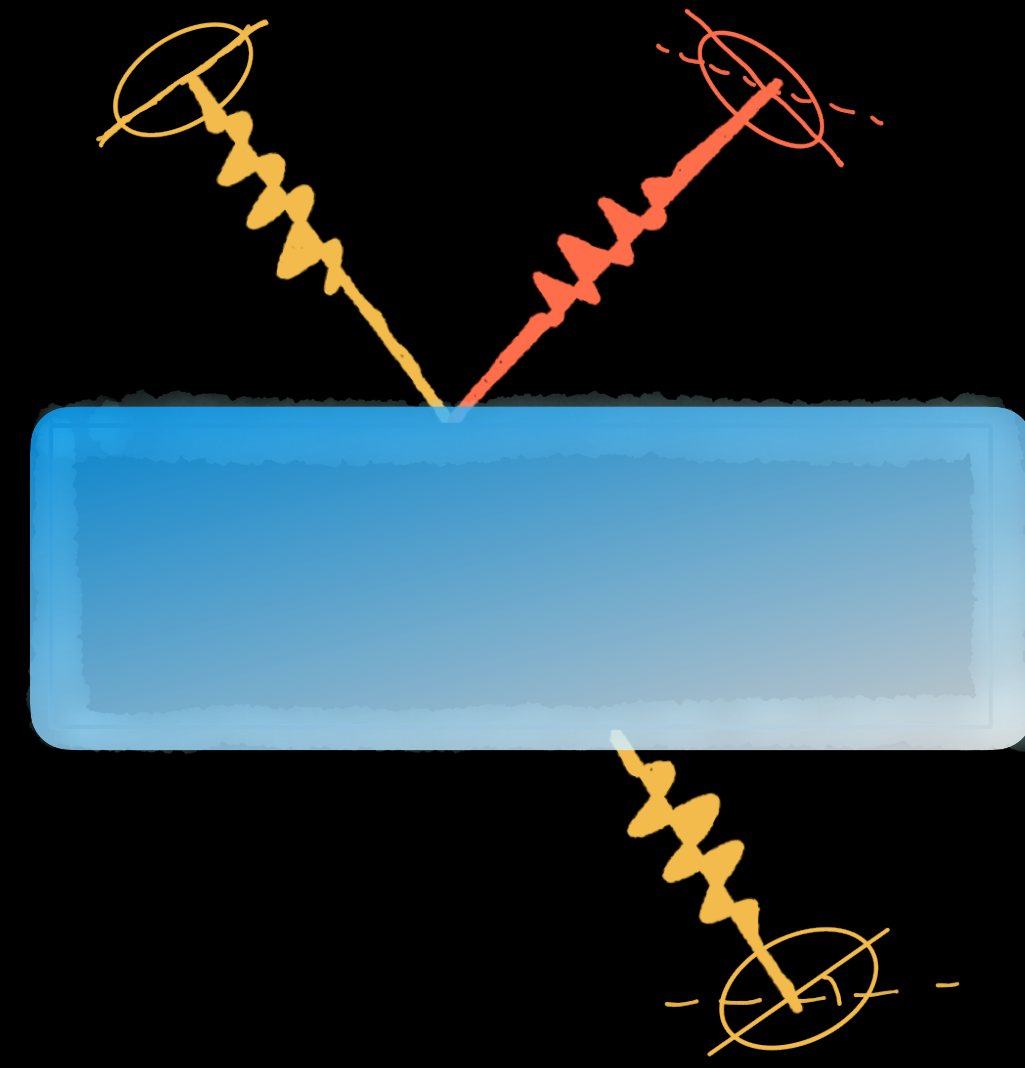
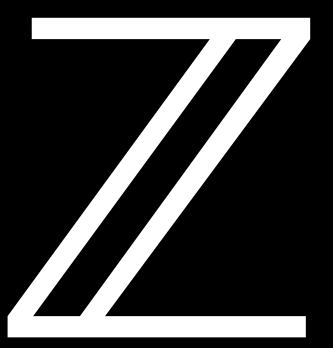
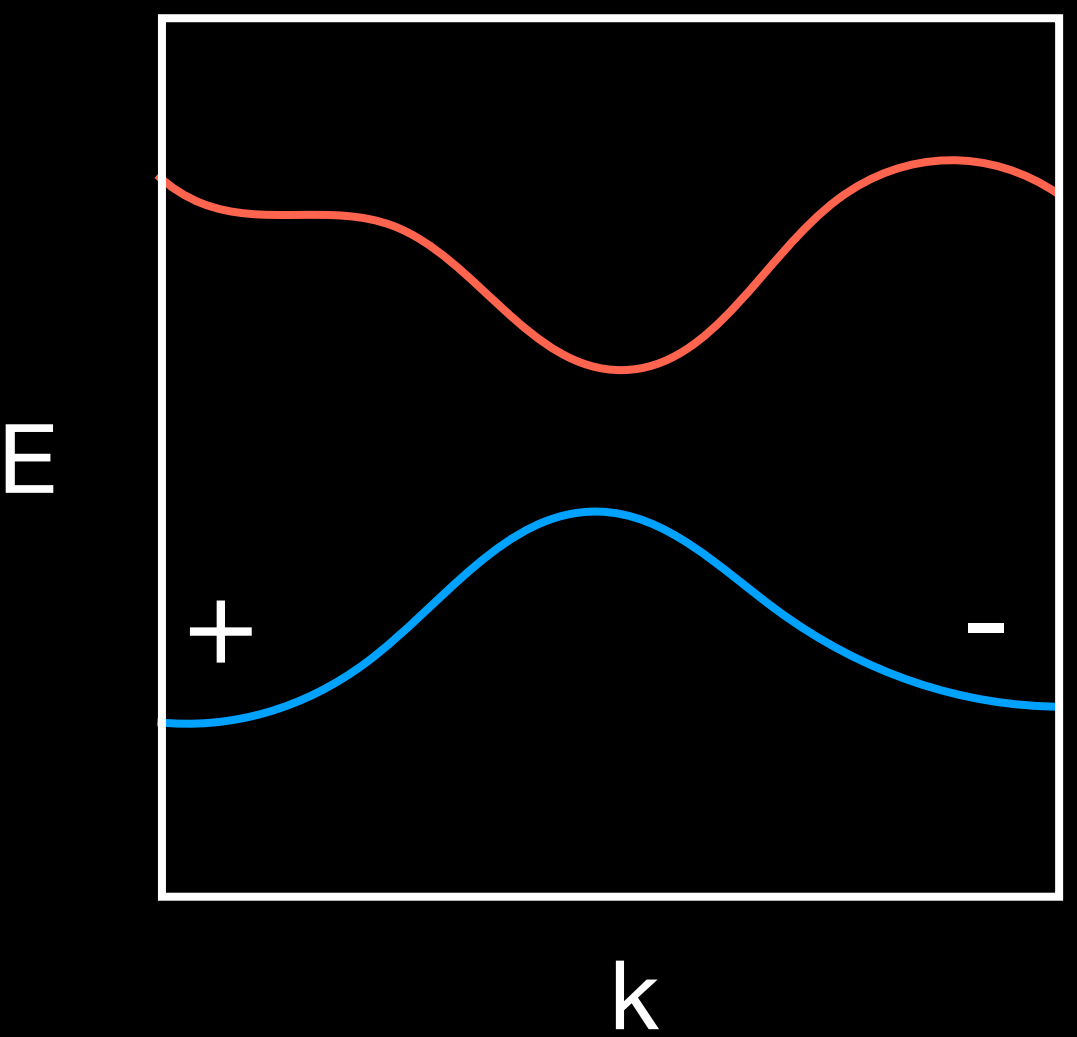
band connectivity + symmetries labels



Topological invariants

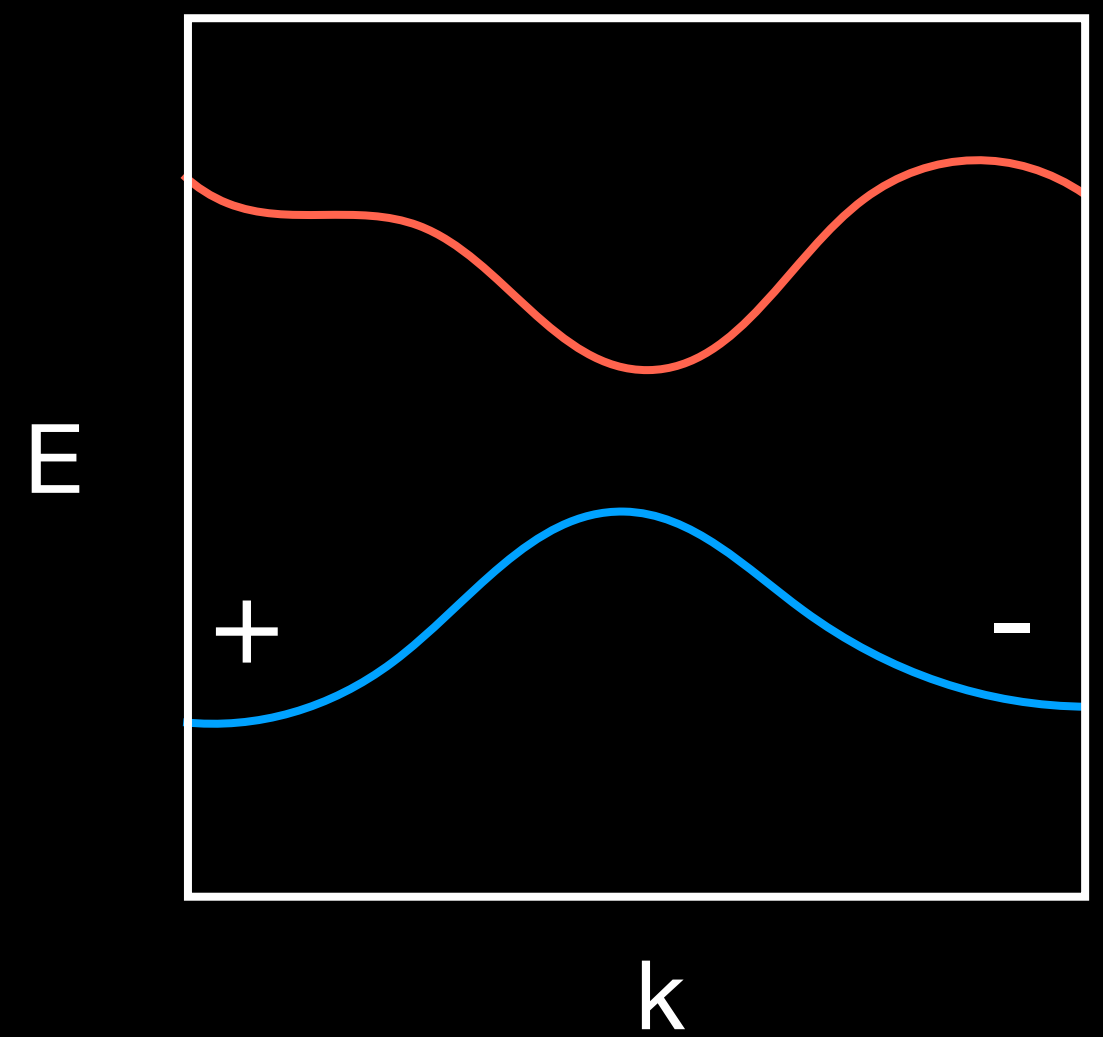


Quantized responses



# How do we find new topological insulators?

band connectivity + symmetries labels



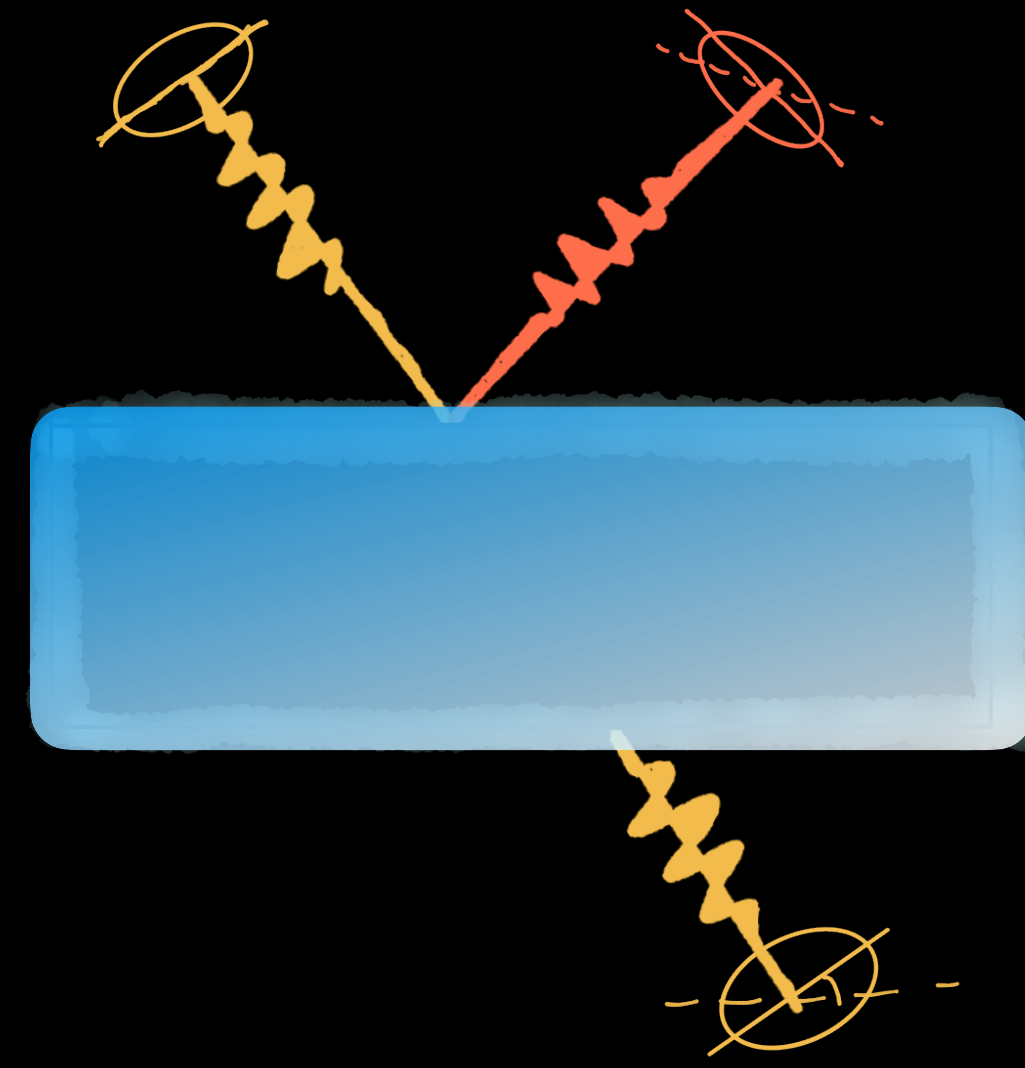
Topological invariants

$$(-1)^\nu = \prod_{\text{TRIM}} \zeta_i$$

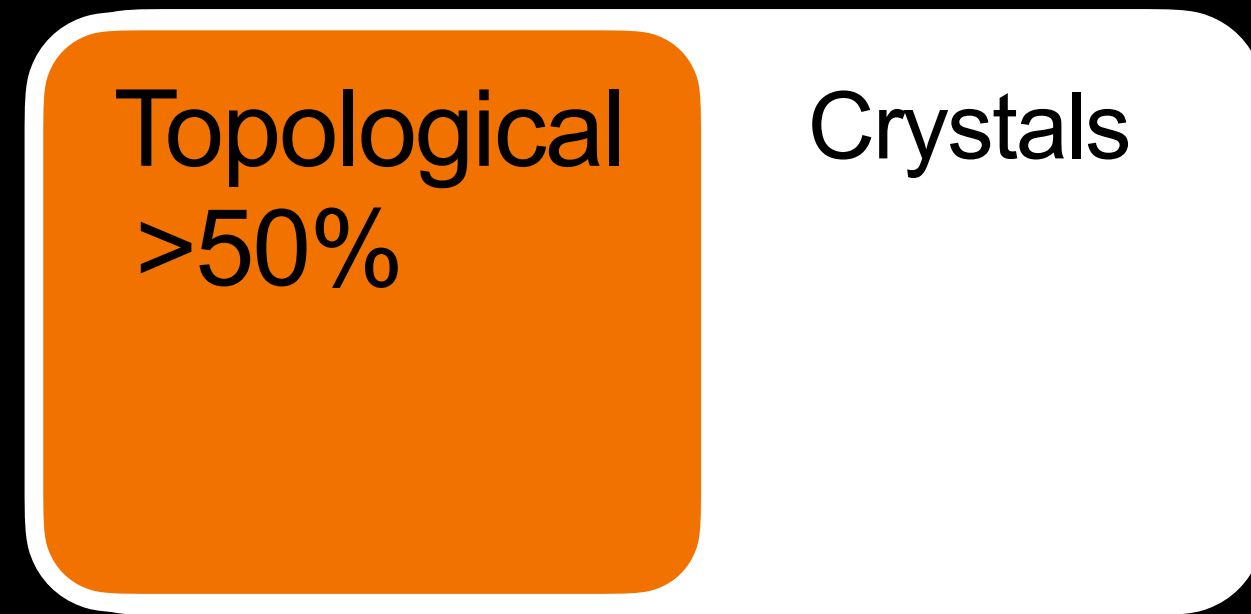
↑  
symmetry eigenvalues



Quantized responses



# Topological solids



Vergniory et al. Nature (2019)

Zhang et al. Nature (2019)

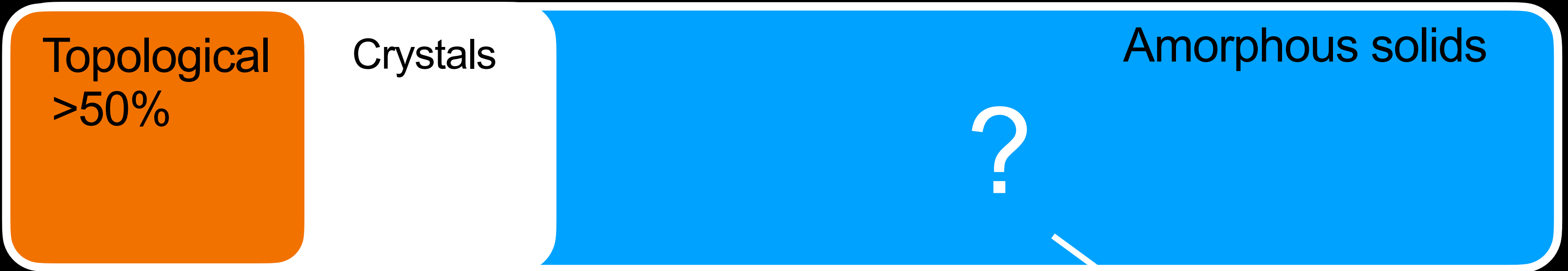
Tang et al. Nature (2019)

# Topological solids

Amorphous > Crystal

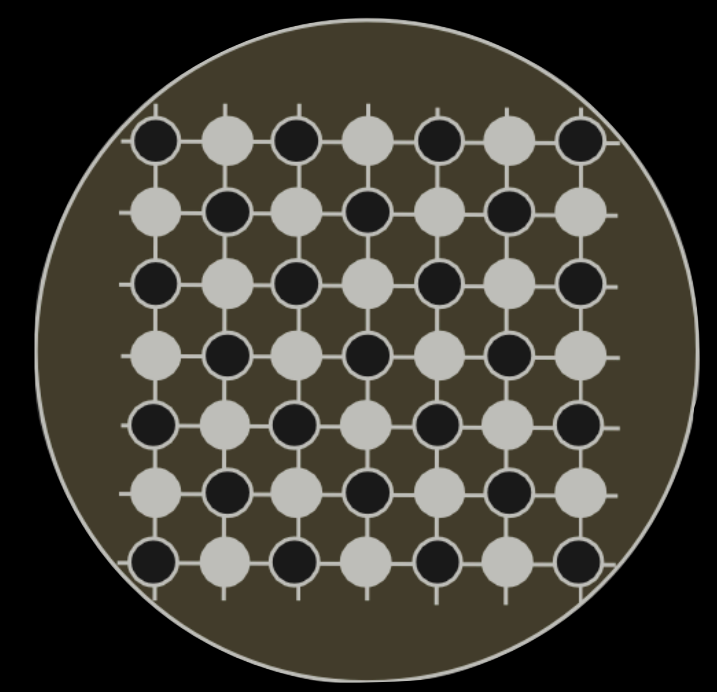
"Nearly all materials can [...] be prepared as amorphous solids"

R. Zallen, *Amorphous Solids*



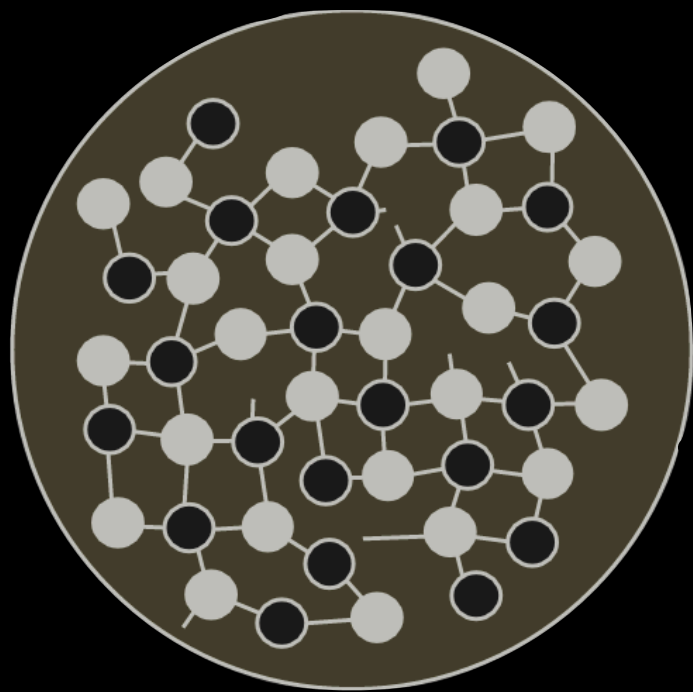
Different capabilities

Cheap and scalable



Crystal

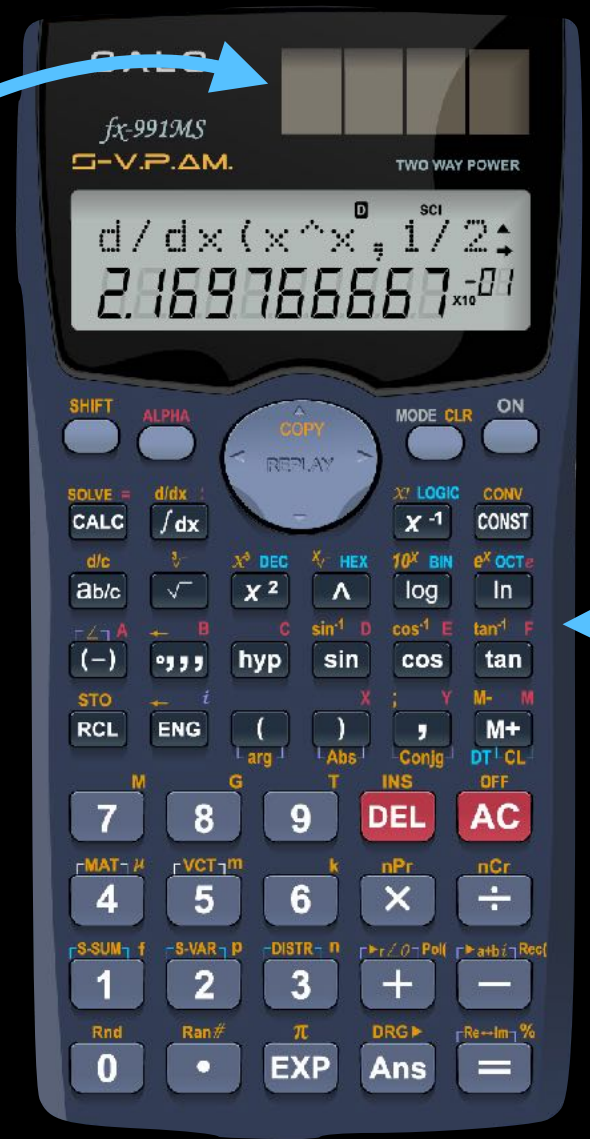
Light or current



Amorphous

Mathias, Naboro Nat Mat (2007)  
Q. Marsal, D. Varjas, AGG Phys Rev B, (2023)

Solar cells

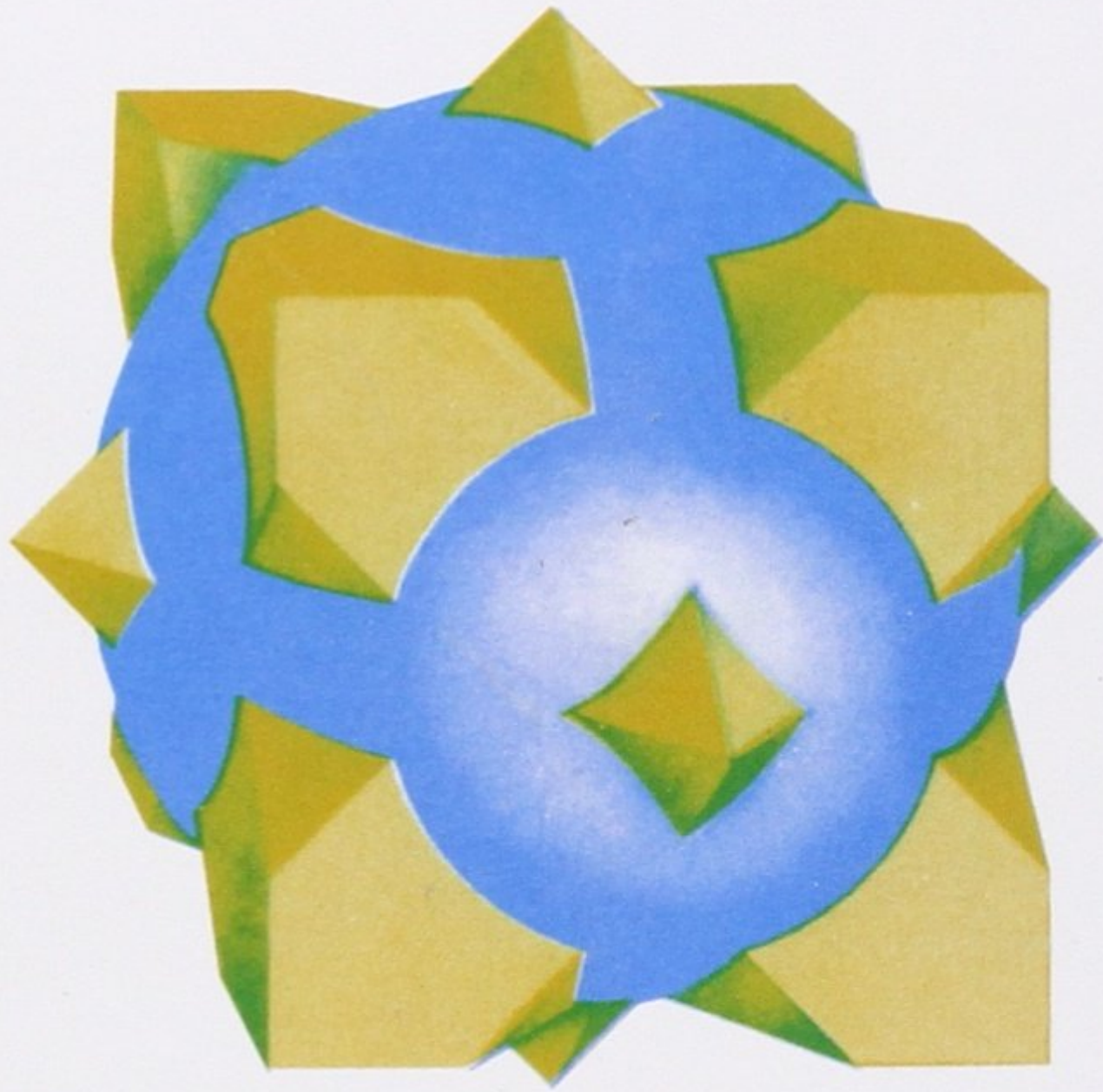


Memories



Why are we missing amorphous solids?

ASHCROFT/ MERMIN



SOLID STATE PHYSICS



Absent in solid-state textbooks (typically)

amorphous solids

topological phases

# How do we find amorphous topological insulators?

Space Group

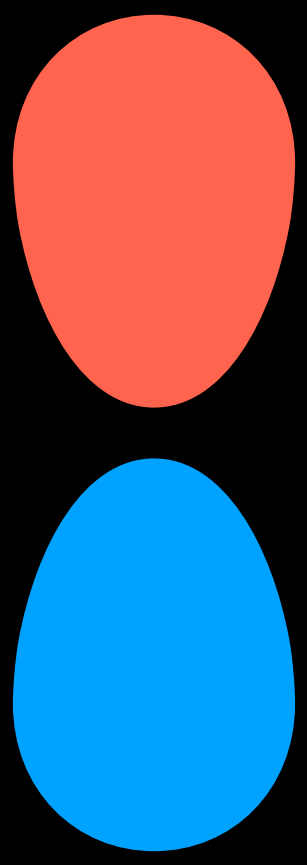


— lattice symmetries

translations, rotations, inversions, mirrors

No long-range order

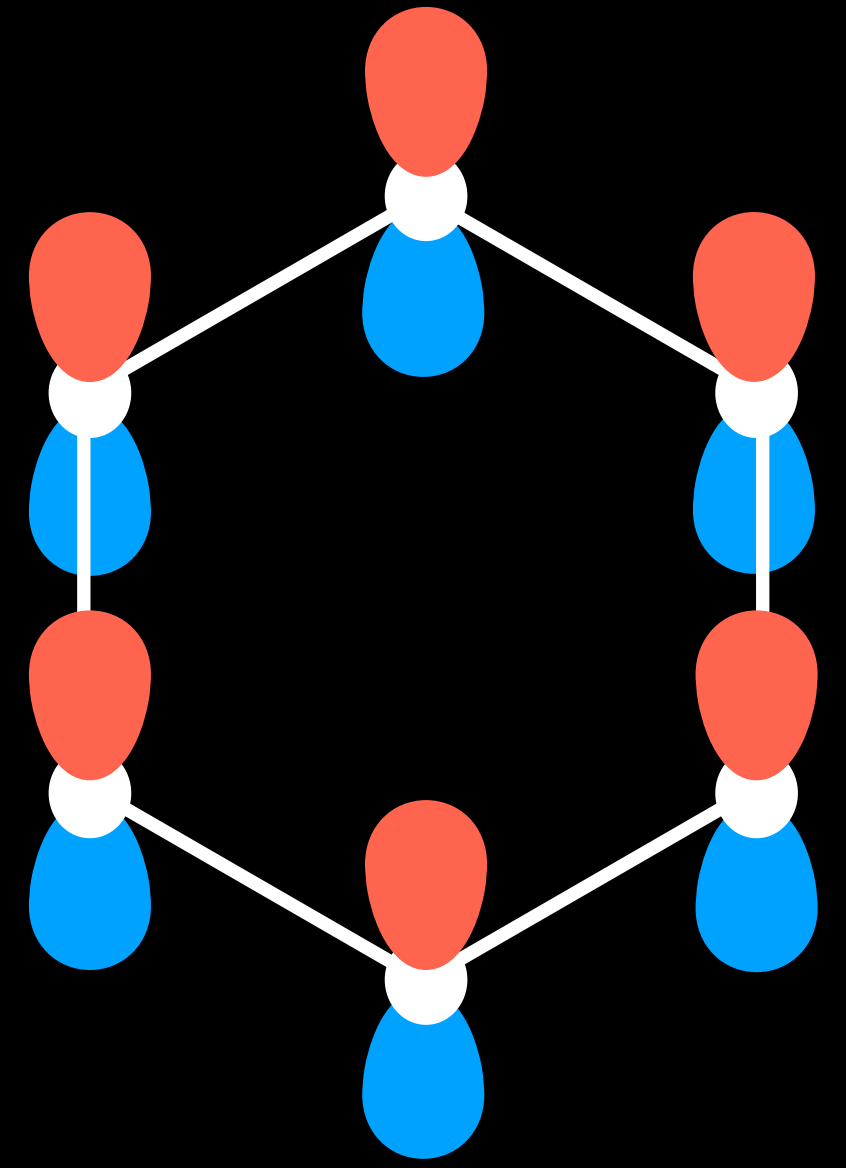
Orbitals



— wavefunctions

s, p, d...

Atomic positions



— band connectivity + symmetries labels

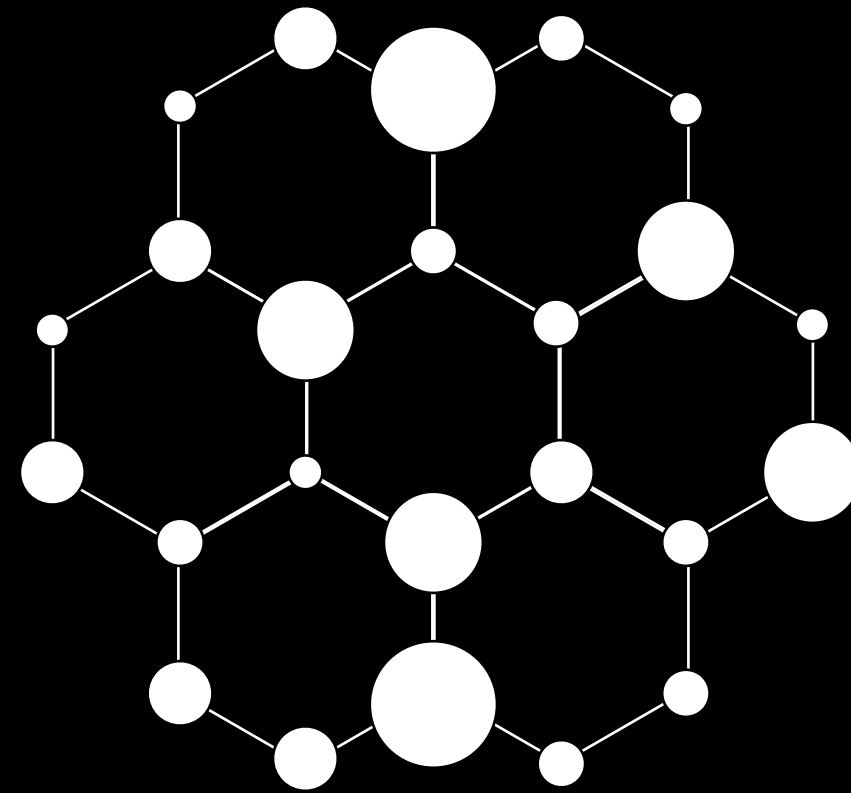
# Topology survives disorder

## Some choices

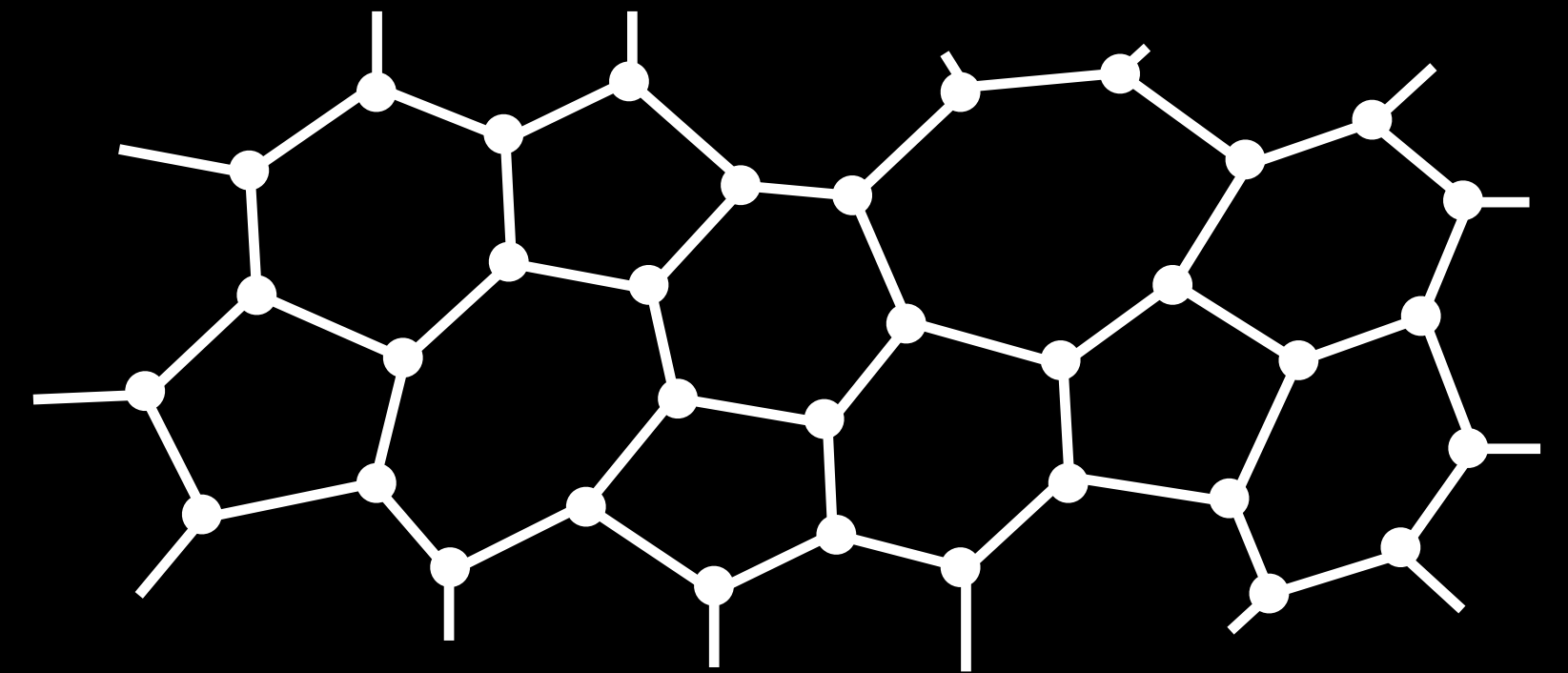
Bond disorder



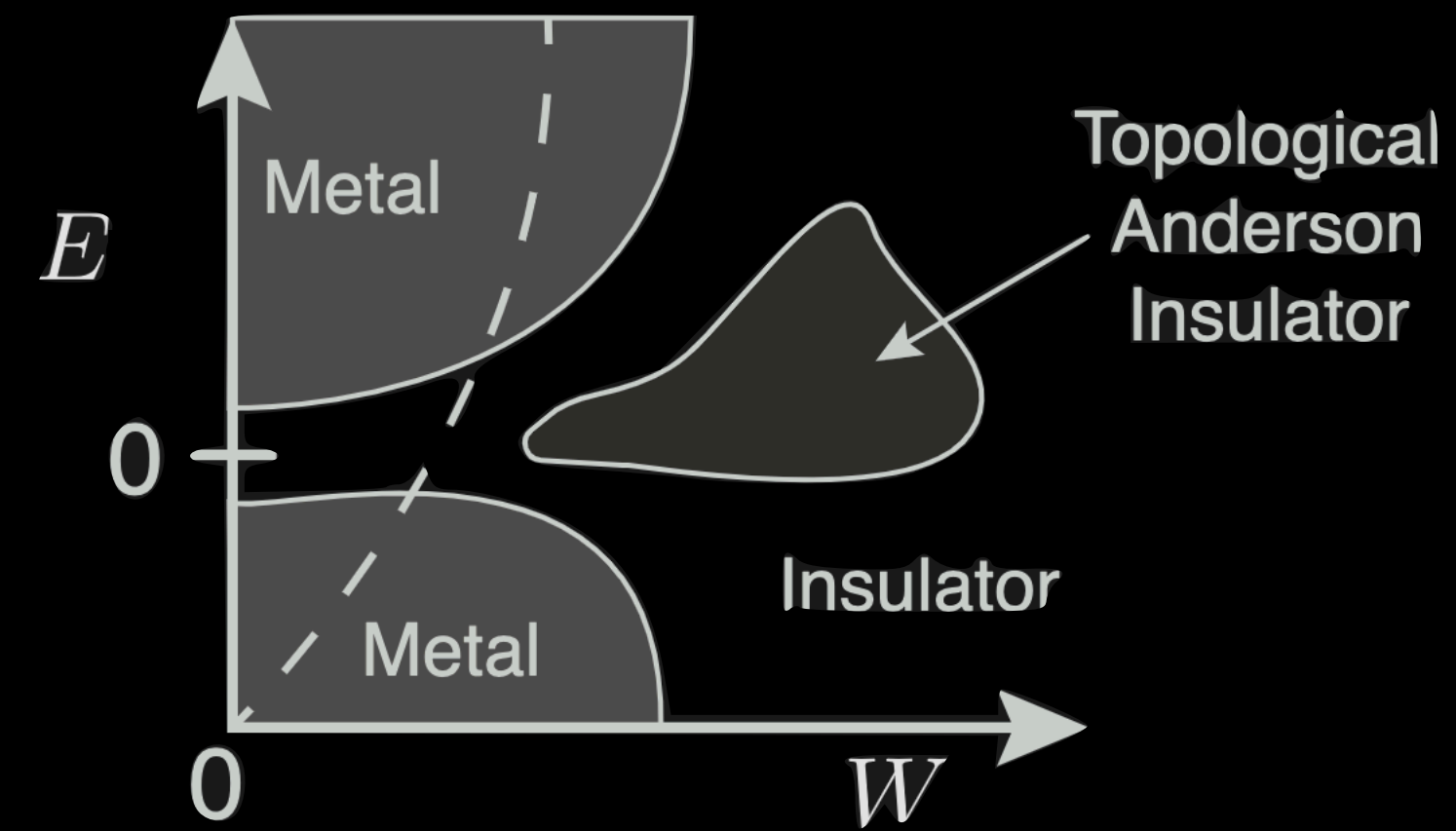
Onsite disorder



Structural disorder

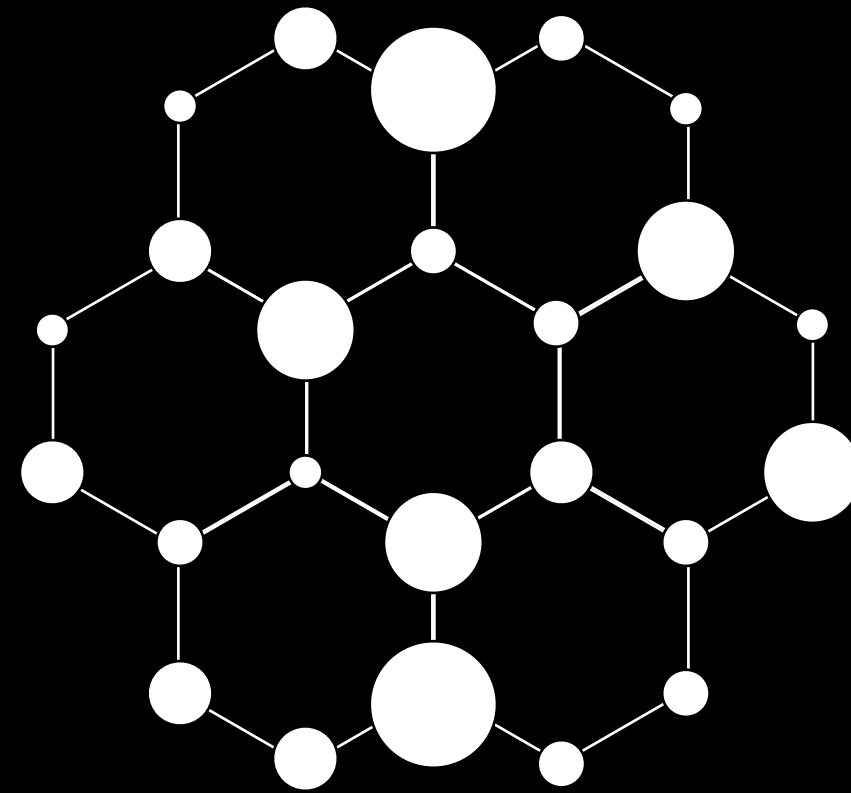


# Topology survives disorder



Li et al PRL (2009)  
Groth et al. PRL (2009)

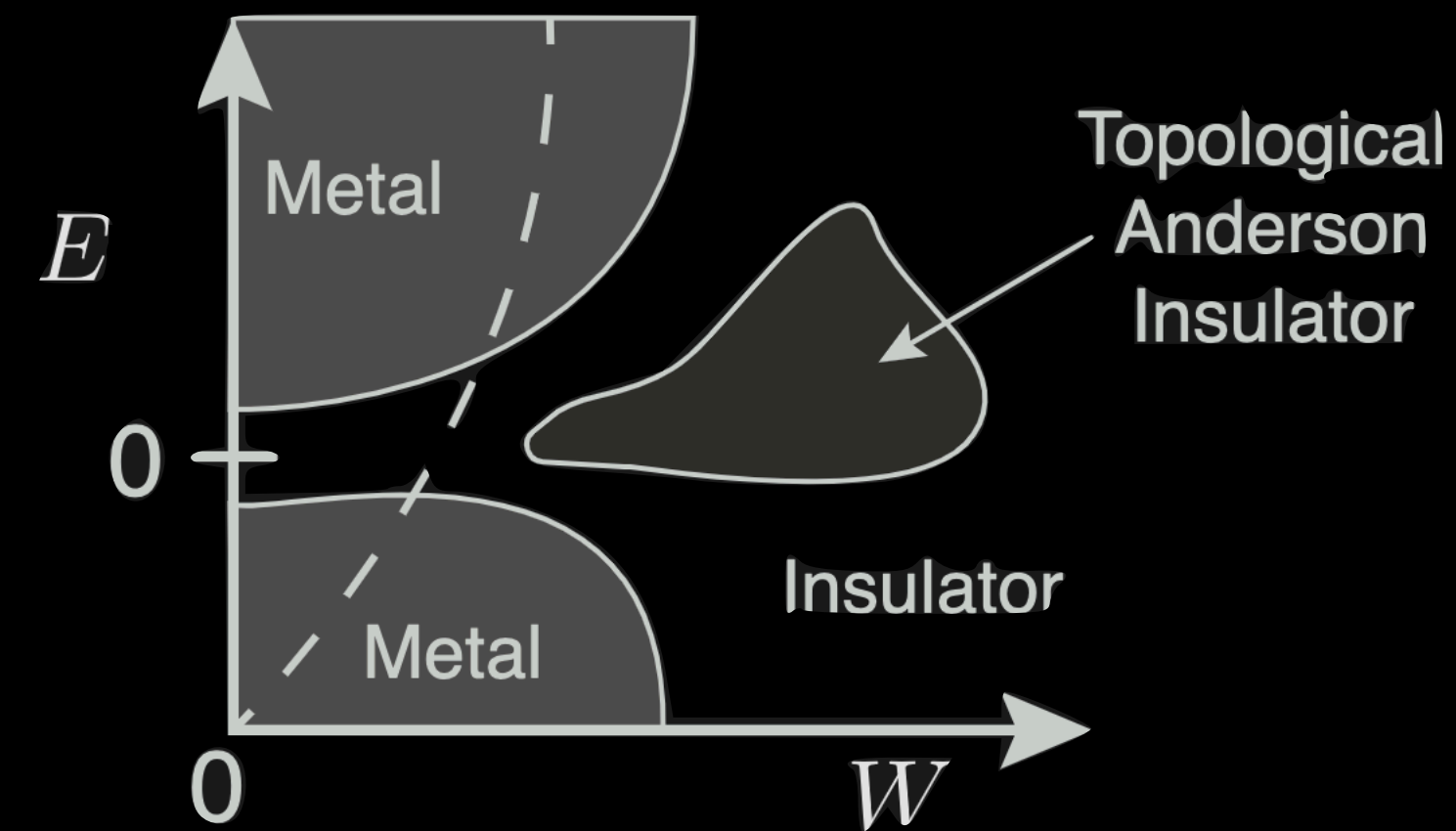
Onsite disorder



# Topology survives disorder

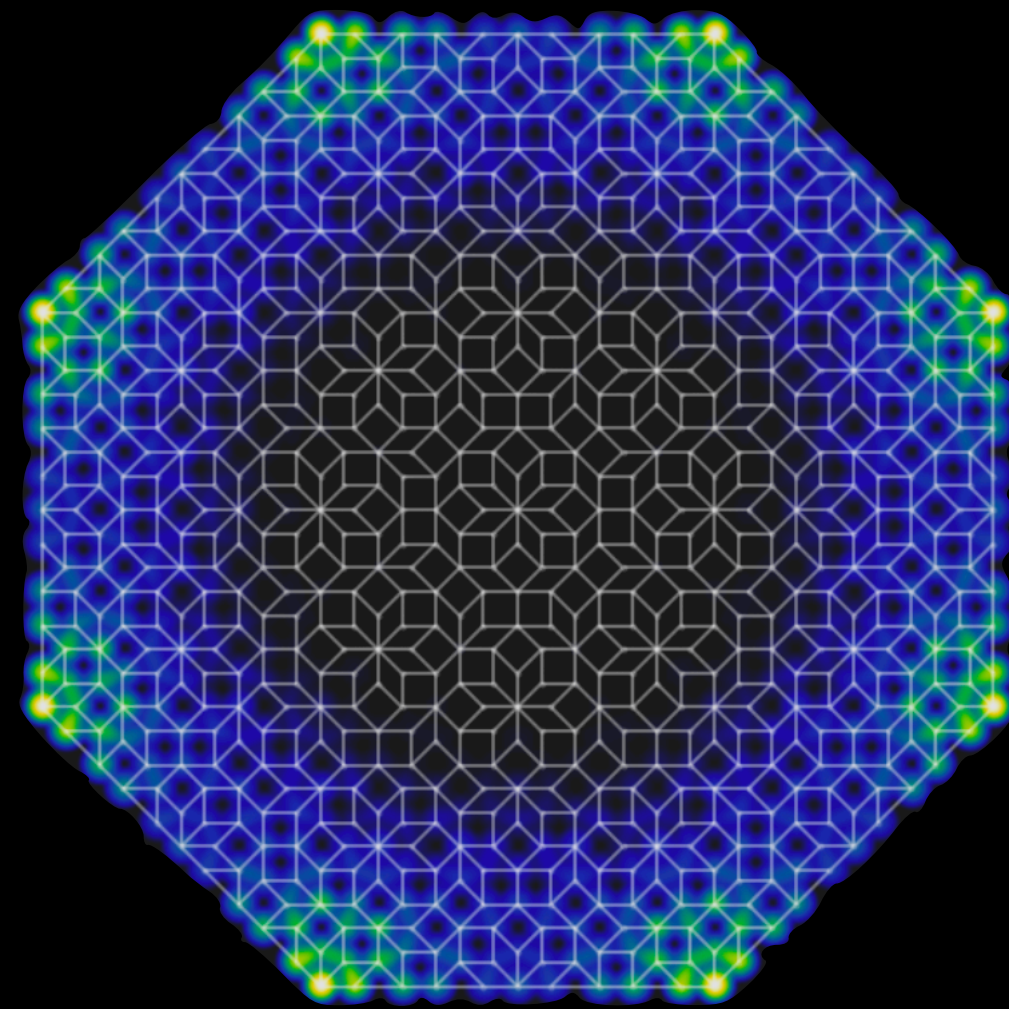
topology is not restricted by translational invariance

Disordered systems



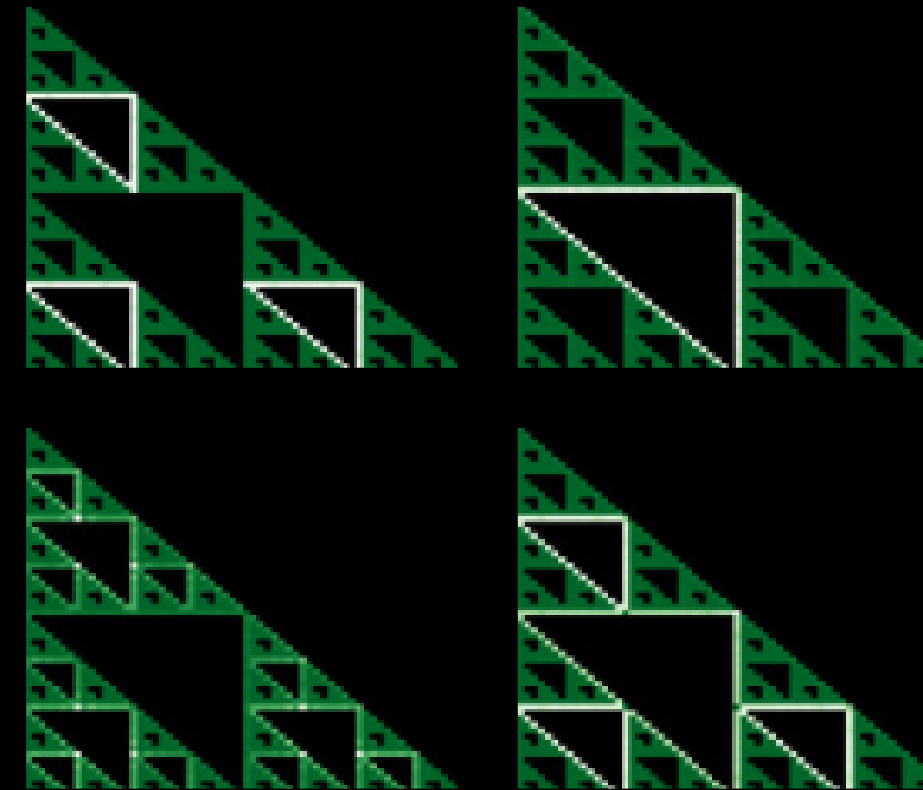
Li et al PRL (2009)  
Groth et al. PRL (2009)

Quasicrystals



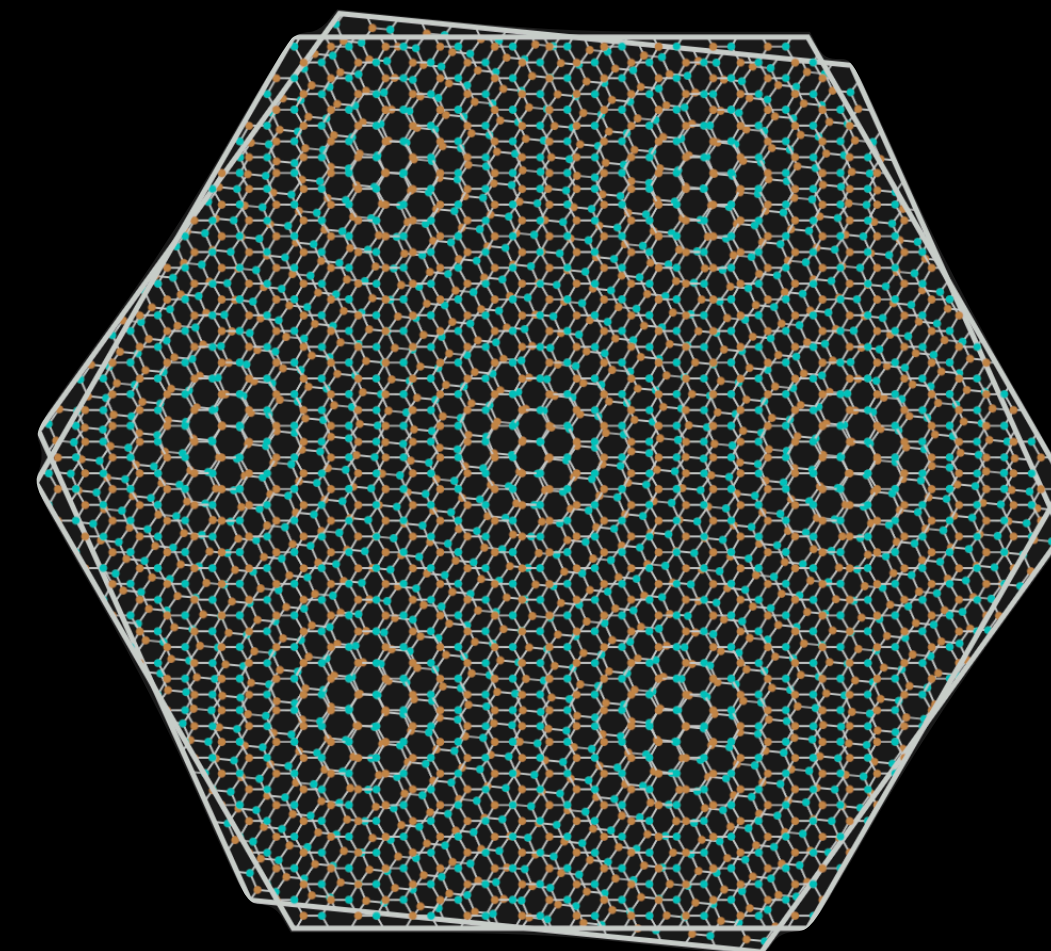
Fuchs and Vidal PRB (2016)  
Varjas et al. PRL (2019)

Fractals



Brzezinska et al. PRB (2018)

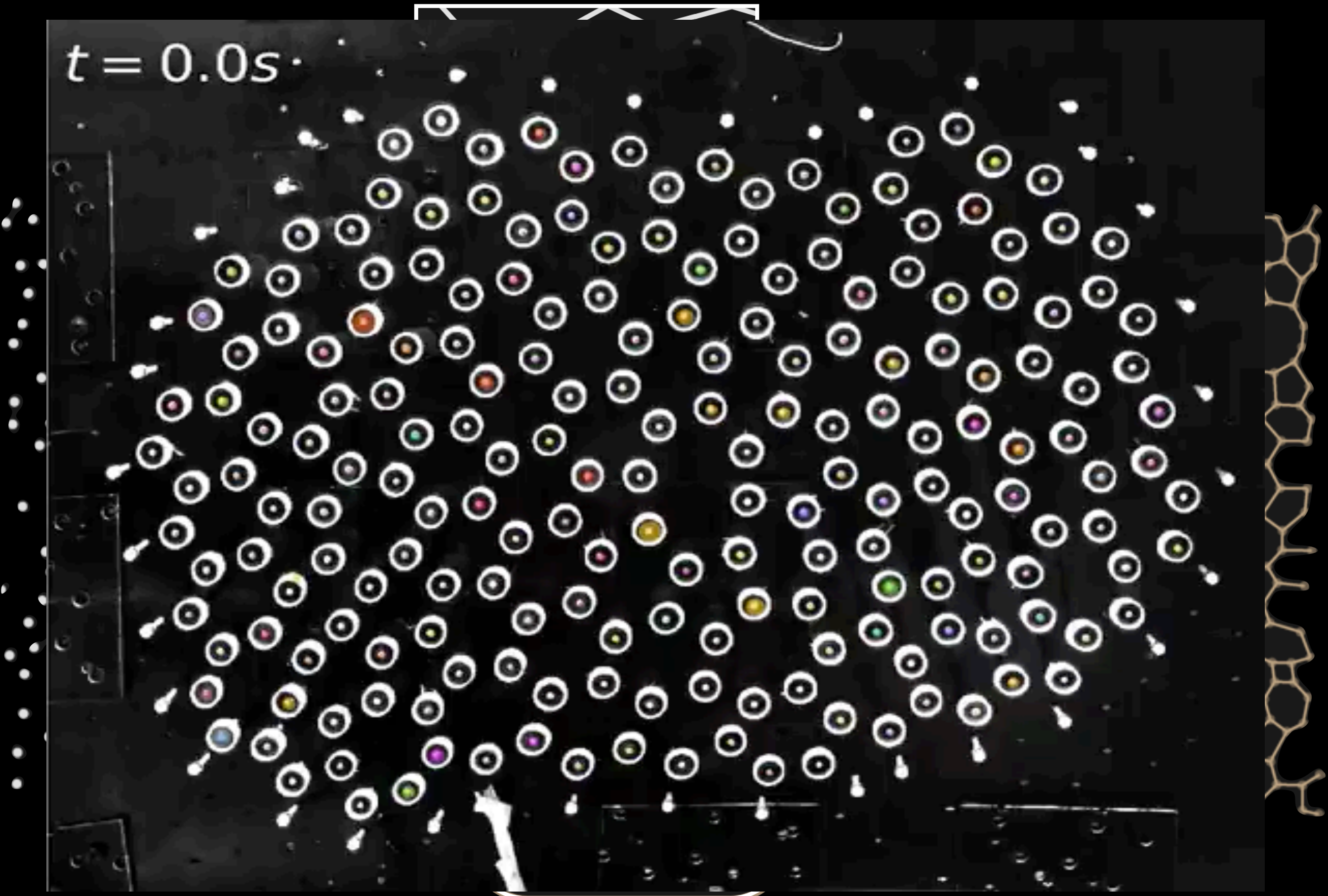
Moiré superlattices



Cao et al. Nature (2018)

# A recent addition: amorphous topological phases

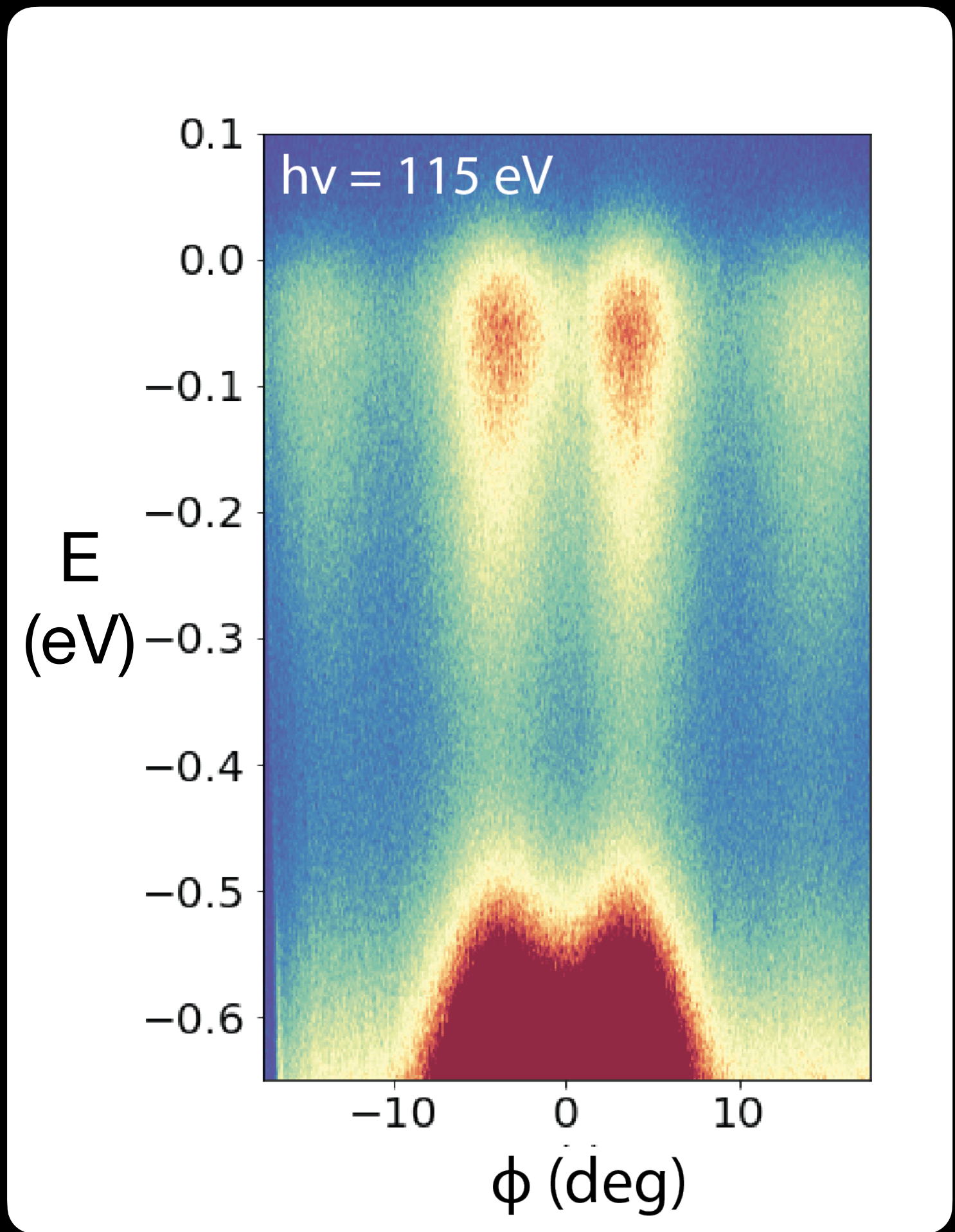
Synthetic systems:



Theory:  
 Agarwala, Shenoy PRL (2017)  
 Xia and Fan PRB (2017)  
 Mansha and Shong PRB (2018)

Exp: Mitchell, et al. Nat Phys (2018)  
 Liu et al PRL (2020)  
 Zhou et al Light: Science and App. (2020)  
 Jia, et al. arXiv: 2211.12719  
 Zhang, et al. Sci. Advances (2023)

solid state: a-Bi<sub>2</sub>Se<sub>3</sub>

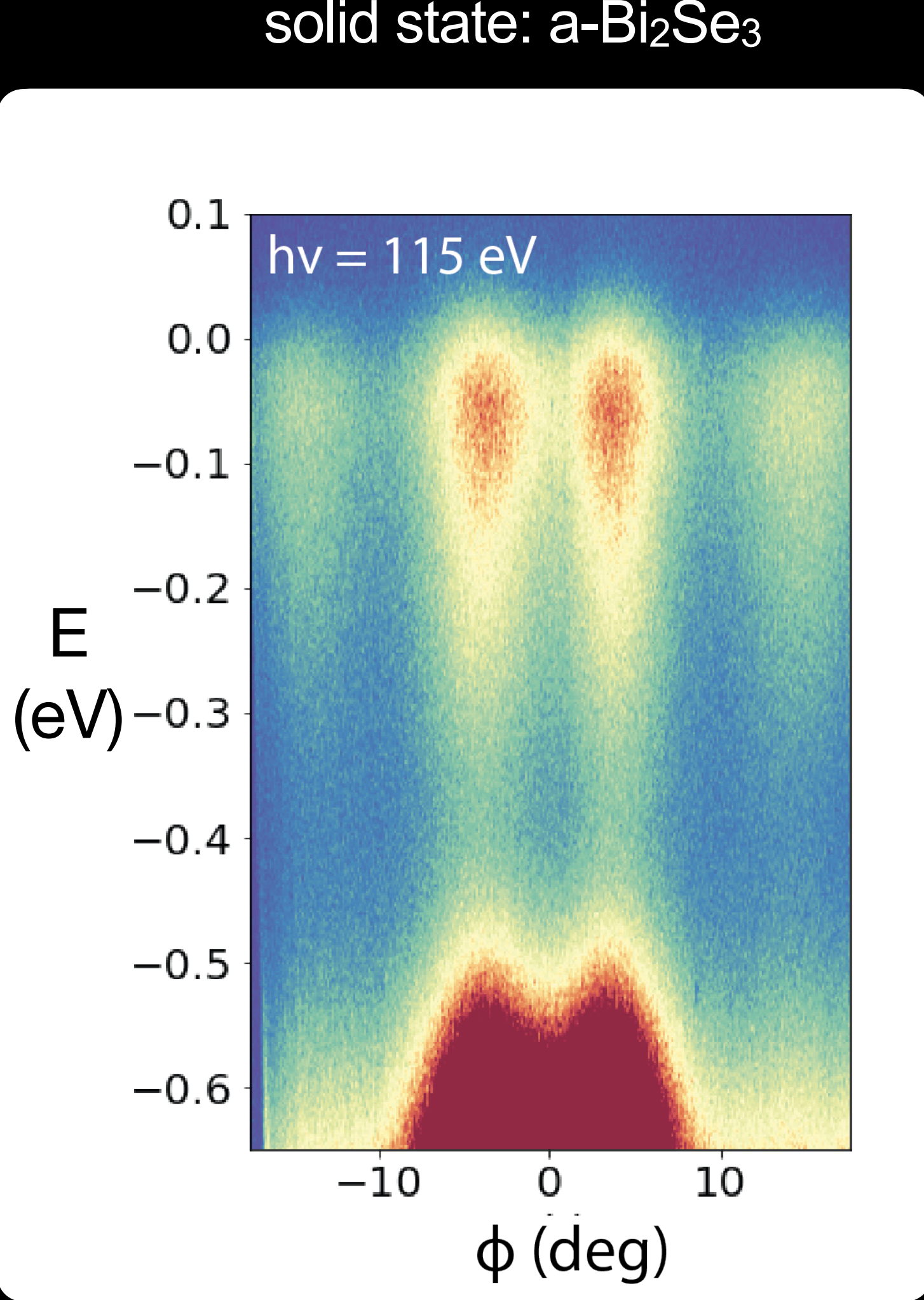


Corbae et al, AGG, Lanzara, Hellmann Nat Materials (2023)  
 Cyocis, Marsal et al, Hellmann, AGG, Lanzara 2302.05945

# Overlooked topological solids?



We just know one!  
= hard to predict



Corbae et al, AGG, Lanzara, Hellmann Nat Materials (2023)  
Cyocis, Marsal et al, Hellmann, AGG, Lanzara 2302.05945



How do we find topological amorphous solids?  
Any different physics compared to crystals?

Amorphous graphene

# Amorphous graphene



# Amorphous graphene



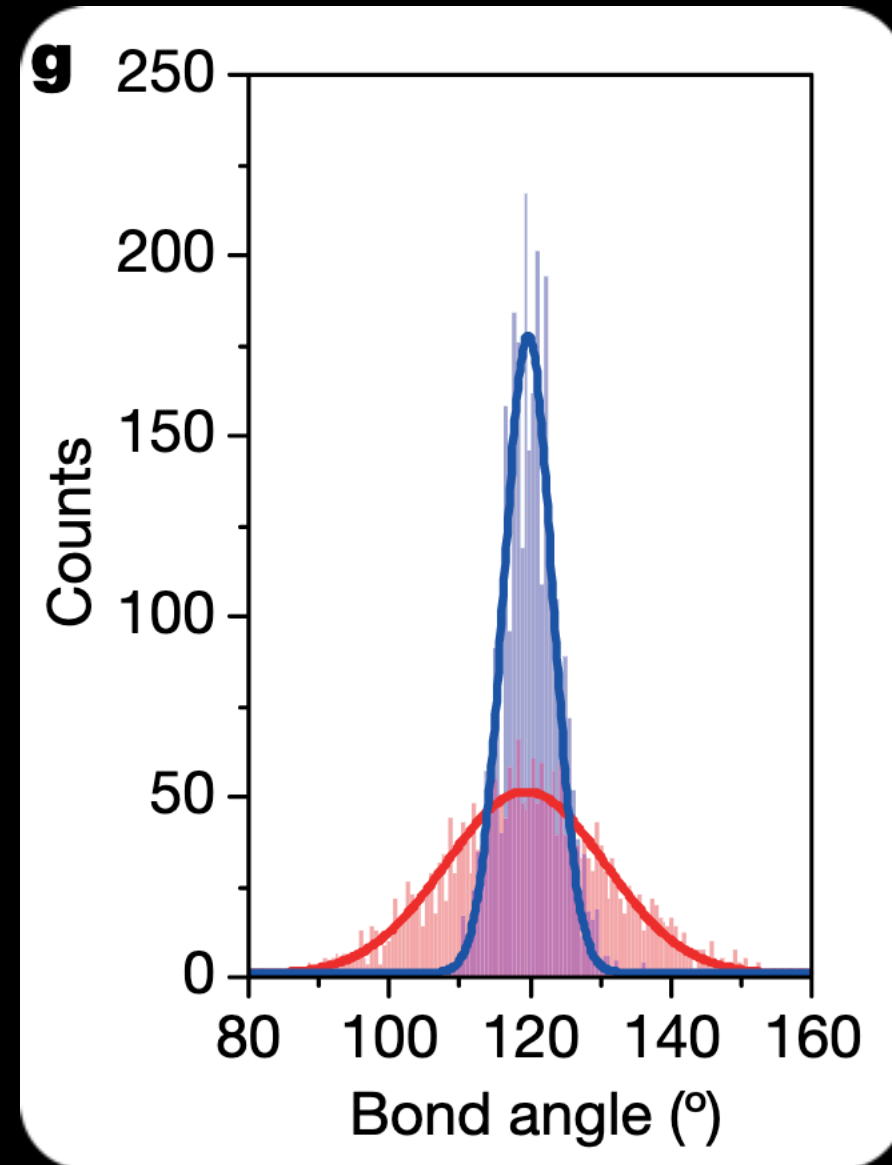
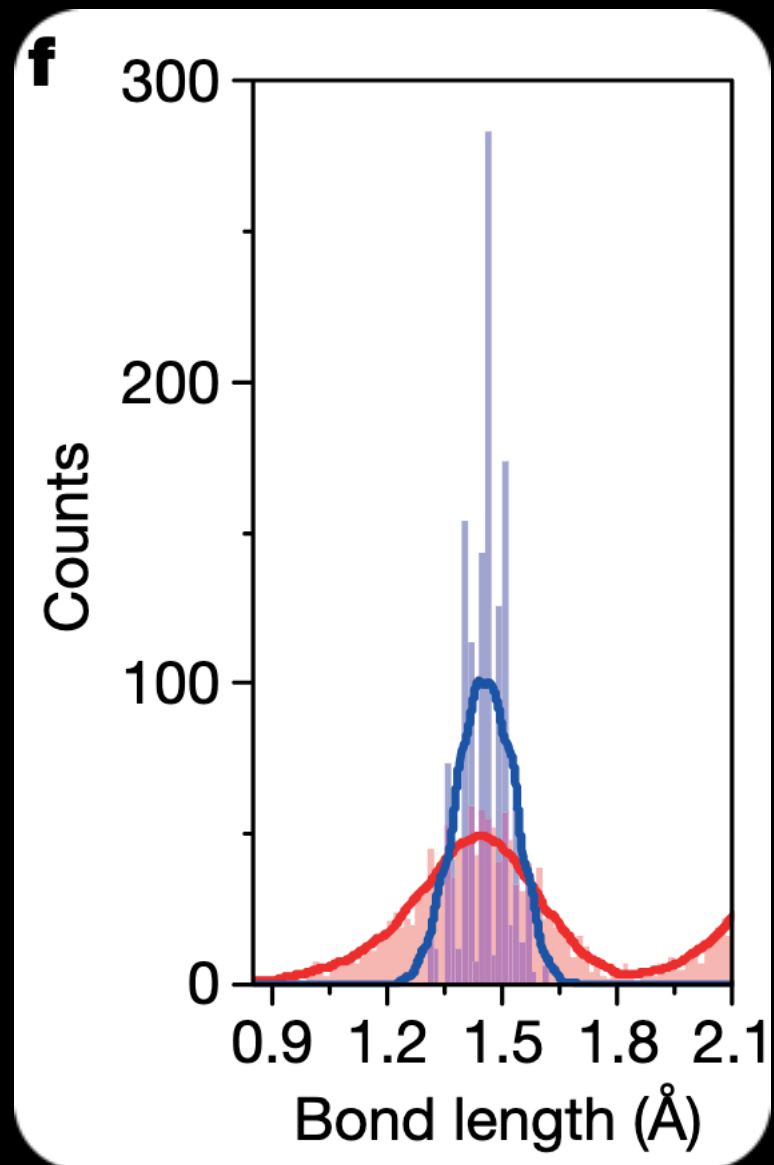
# Amorphous graphene

Local order

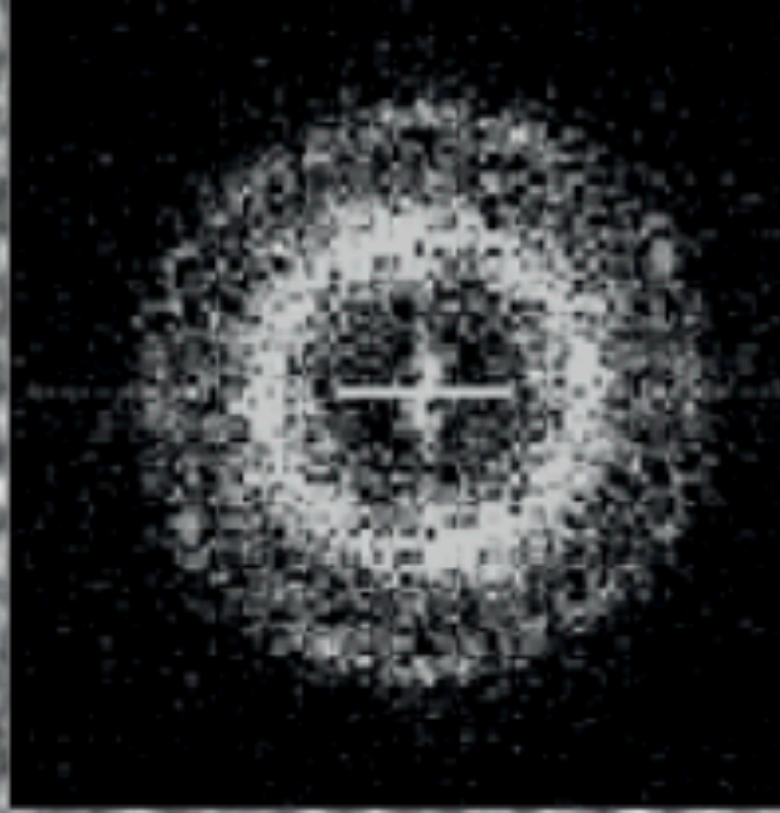
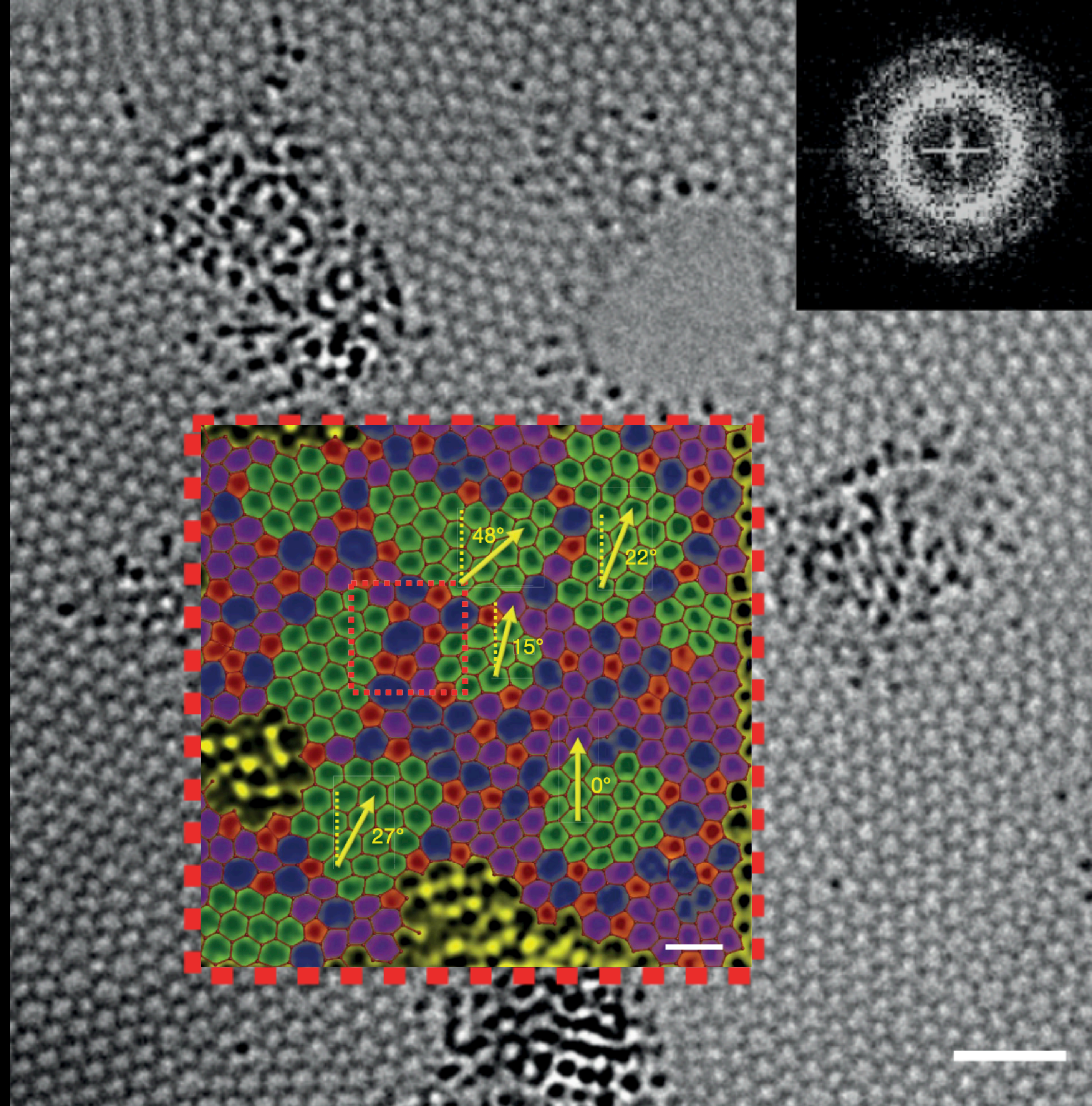
Fixed coordination

Bond lengths

Bond-angles



Crystalline and amorphous regions coexist



What's new?

## Flat-band switch

Q. Marsal, D. Varjas, *AGG Phys Rev B*, (2023)



Quentin Marsal  
Néel Institute



Daniel Varjas  
MPI PKS

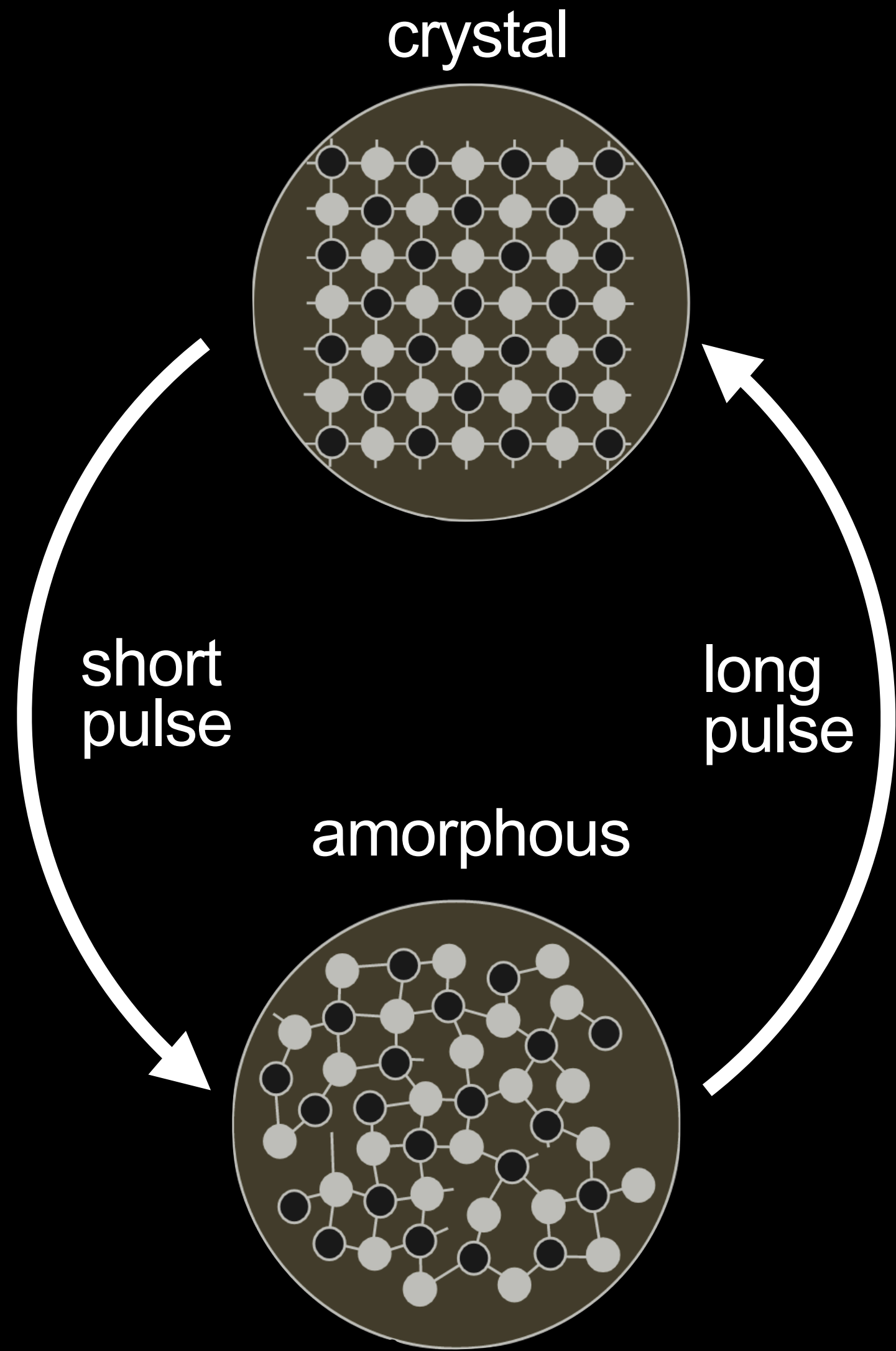
## Amorphous chiral spin-liquid

AGG, C. Repellin 2210.13548



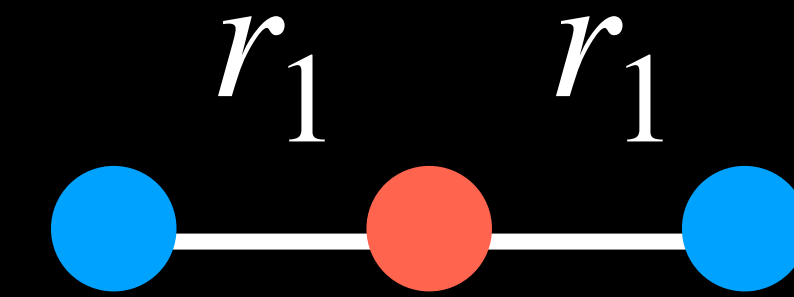
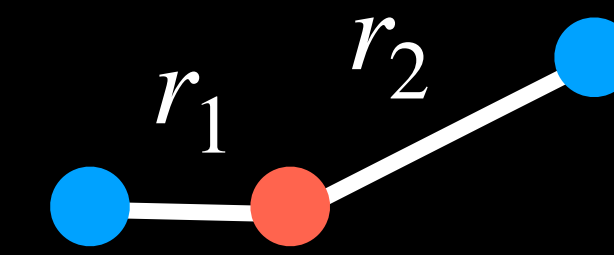
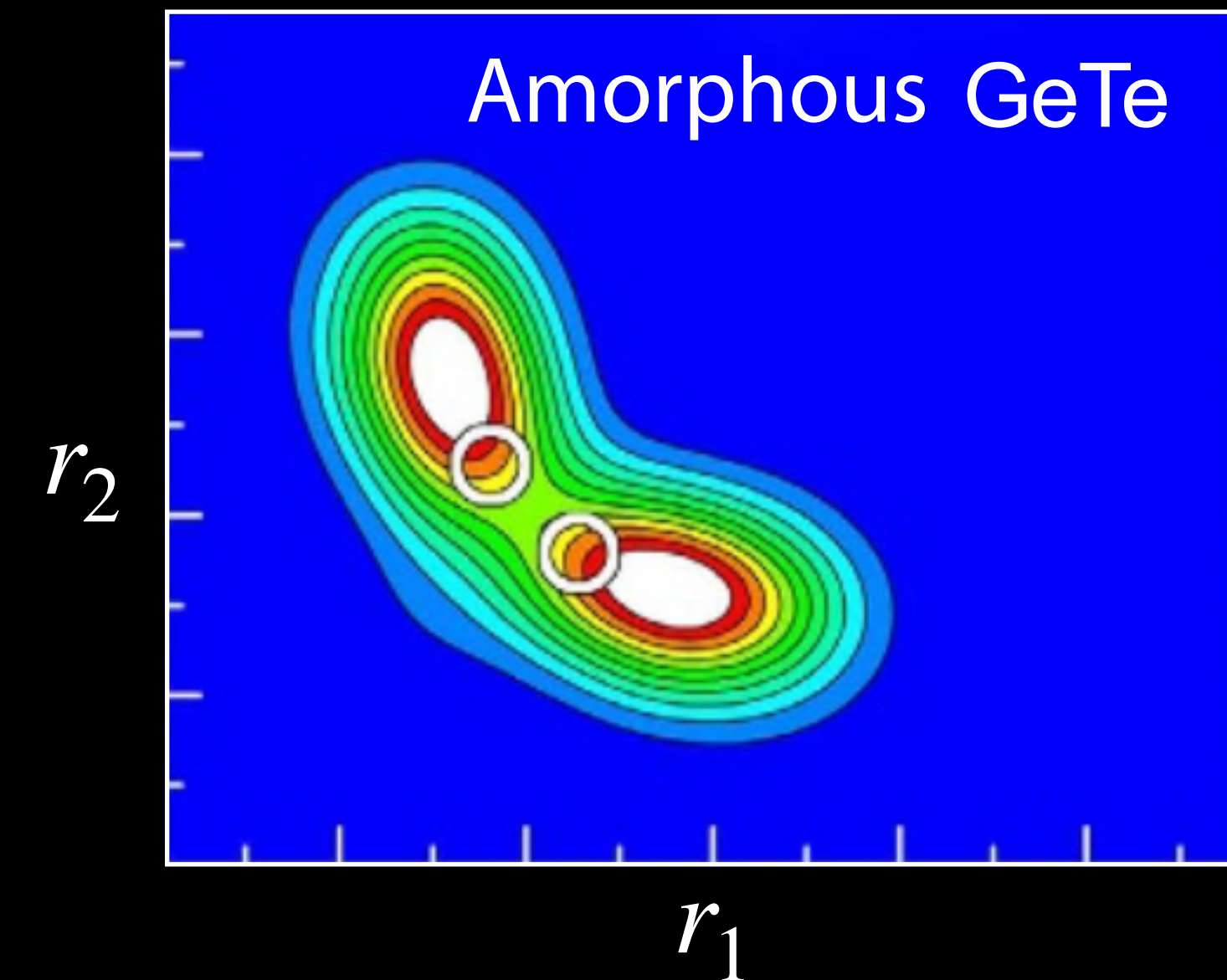
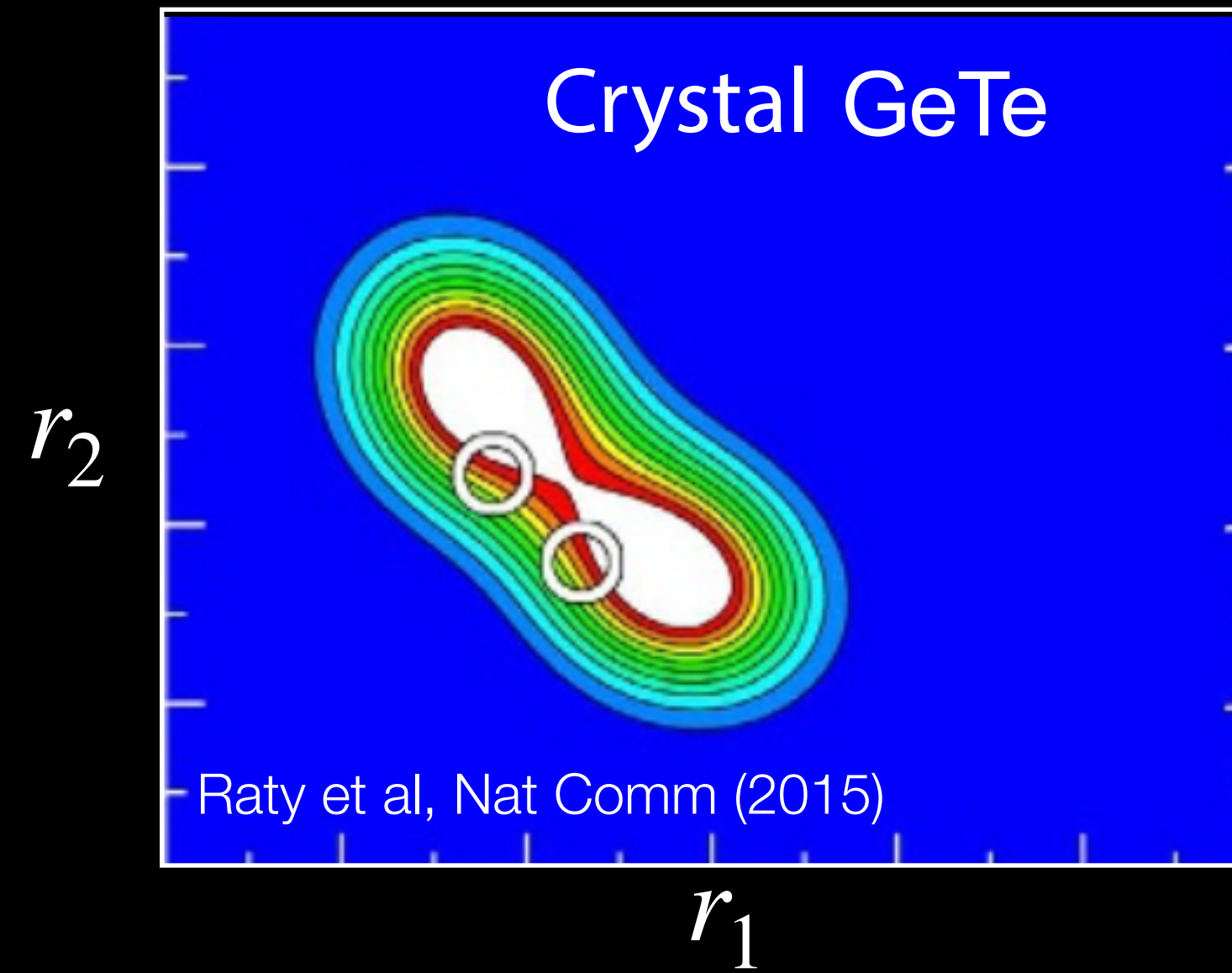
Cécile Repellin  
LPMMC / Grenoble

# Phase-change materials

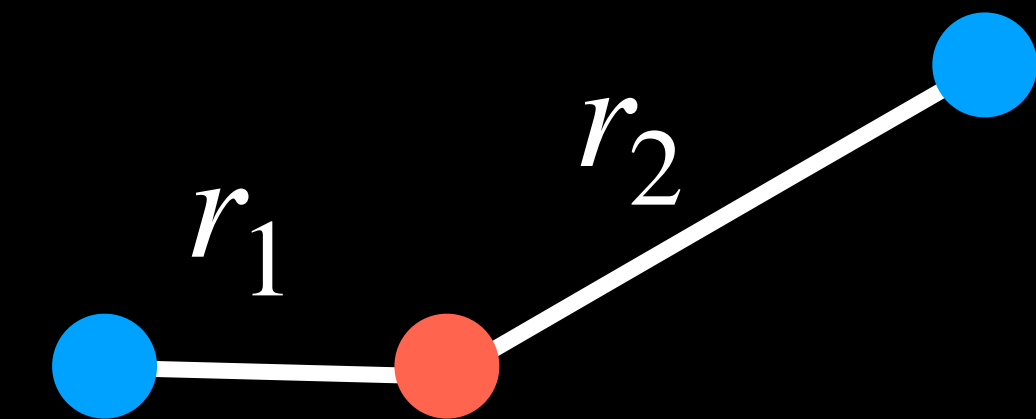


Mathias, Naboro Nat Mat (2007)

## Pair distribution function



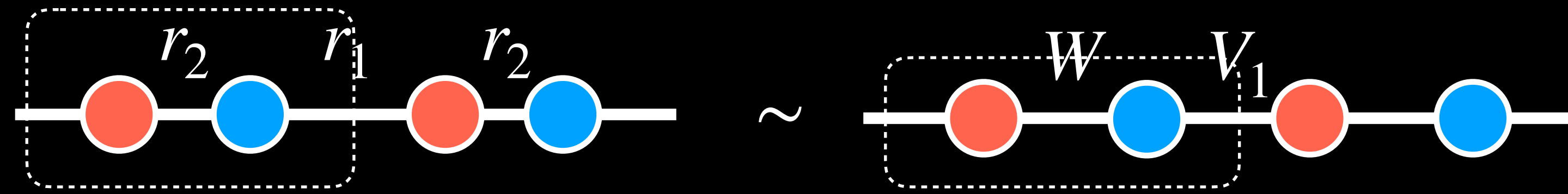
No Peierls distortion



Average Peierls distortion

Gaspard, Comptes Rendus Physique (2016)

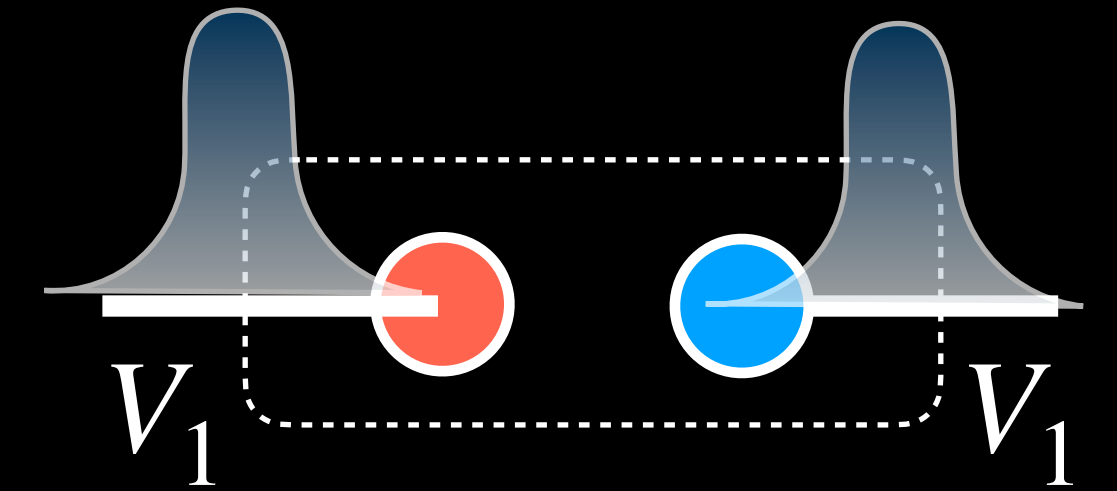
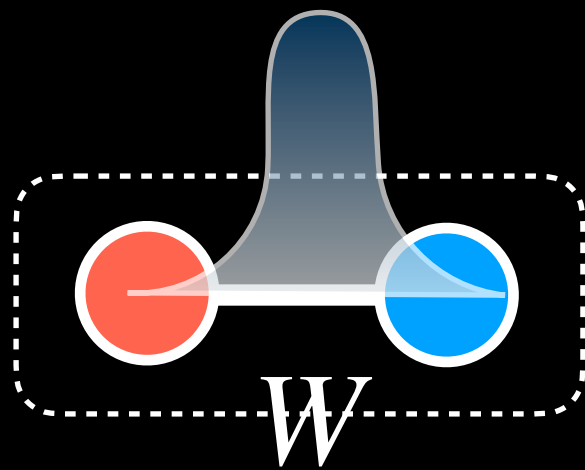
# 1D Peierls phase (SSH)



$$W \gg V_1$$

Two atomic limits

$$W \ll V_1$$



Can't be deformed into each other while preserving gap and inversion

= obstructed atomic limits

Peierls (1955)

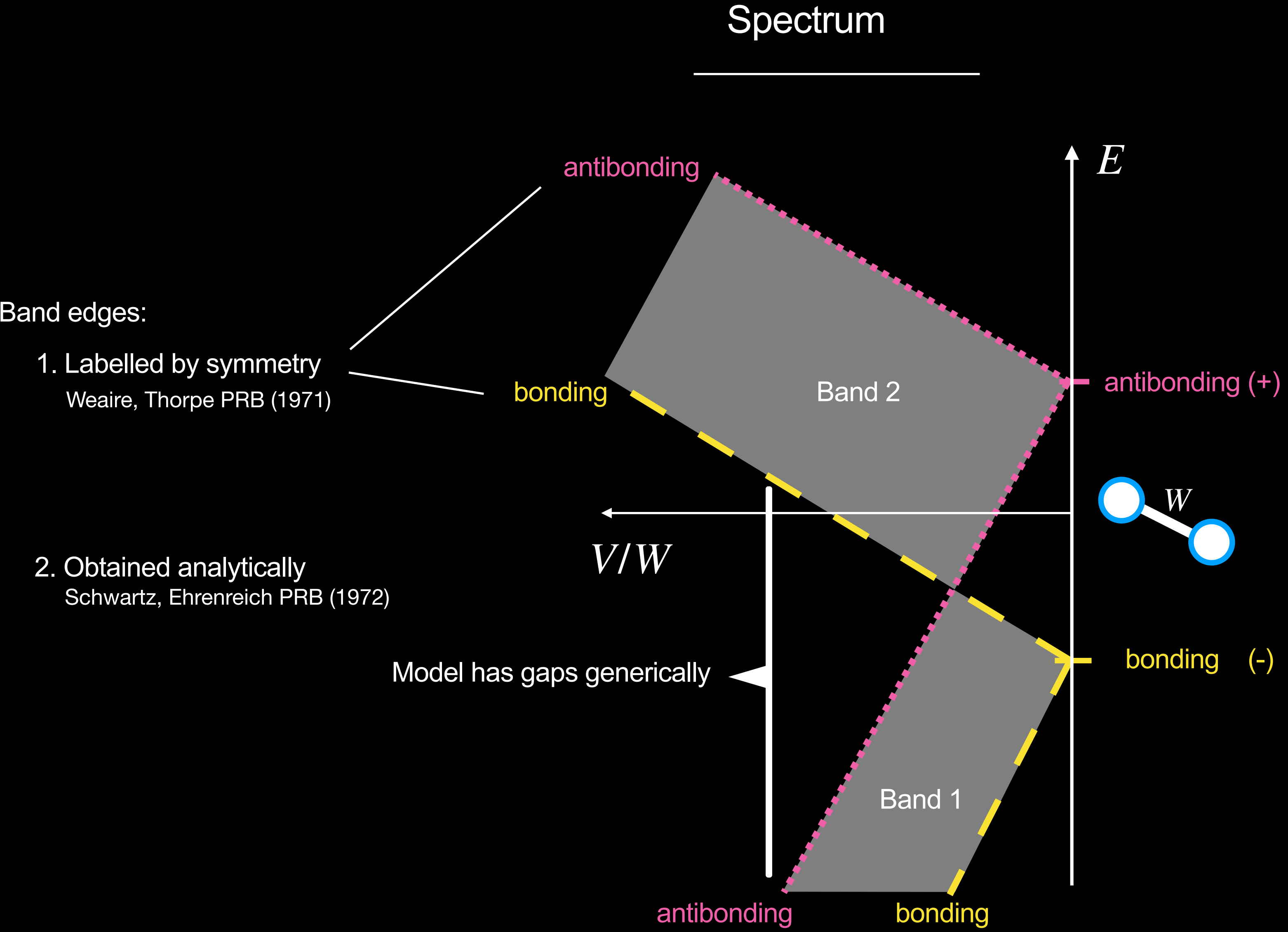
Su, Schrieffer and Heeger PRL (1979)

Song et al PRL (2017), Xu et al 2106.10276



# Fixed coordination = symmetry indicators

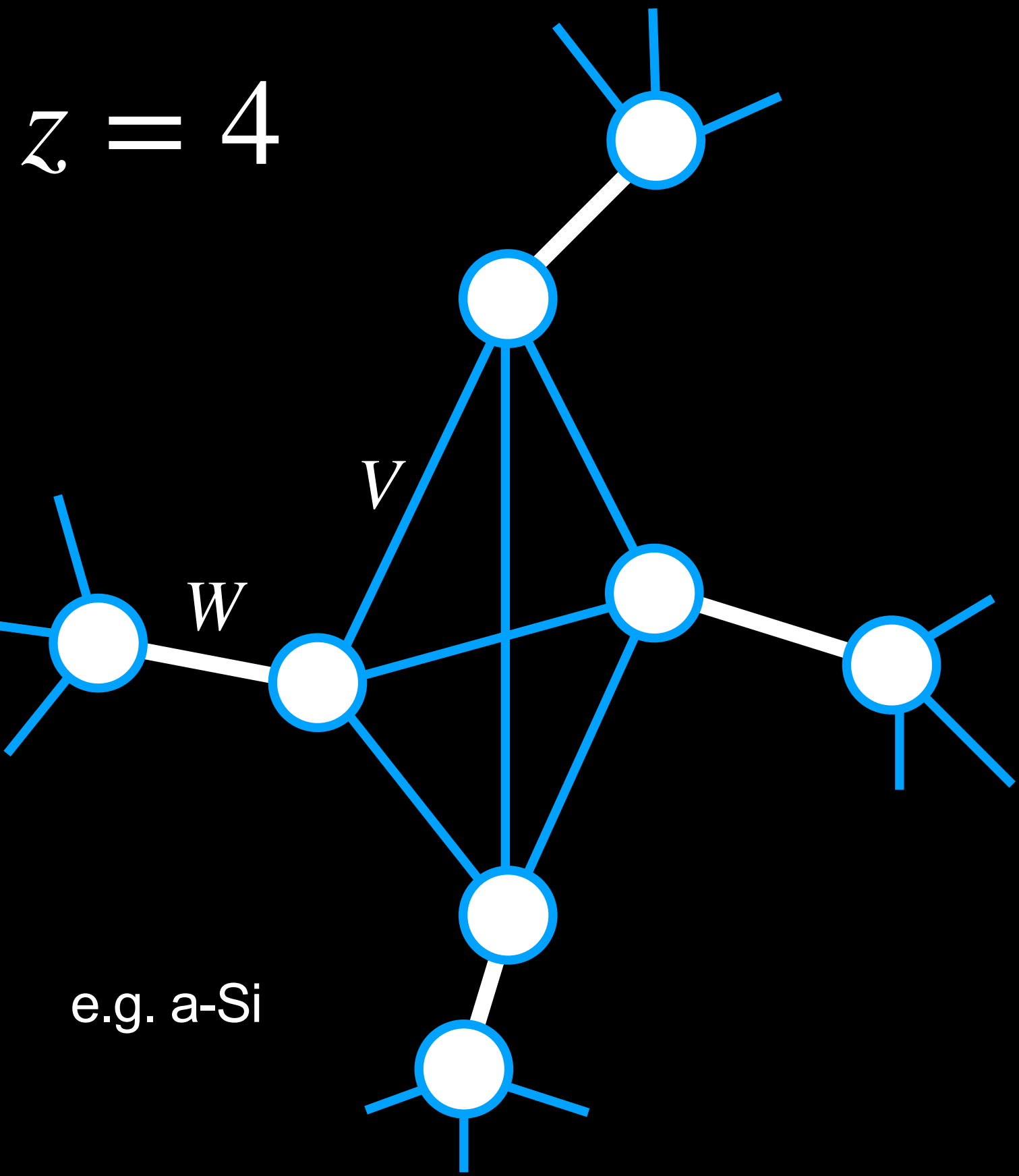
Q. Marsal, D. Varjas, AGG PNAS, (2020)



Band edges:  
1. Labelled by symmetry  
Weaire, Thorpe PRB (1971)

2. Obtained analytically  
Schwartz, Ehrenreich PRB (1972)

Model has gaps generically

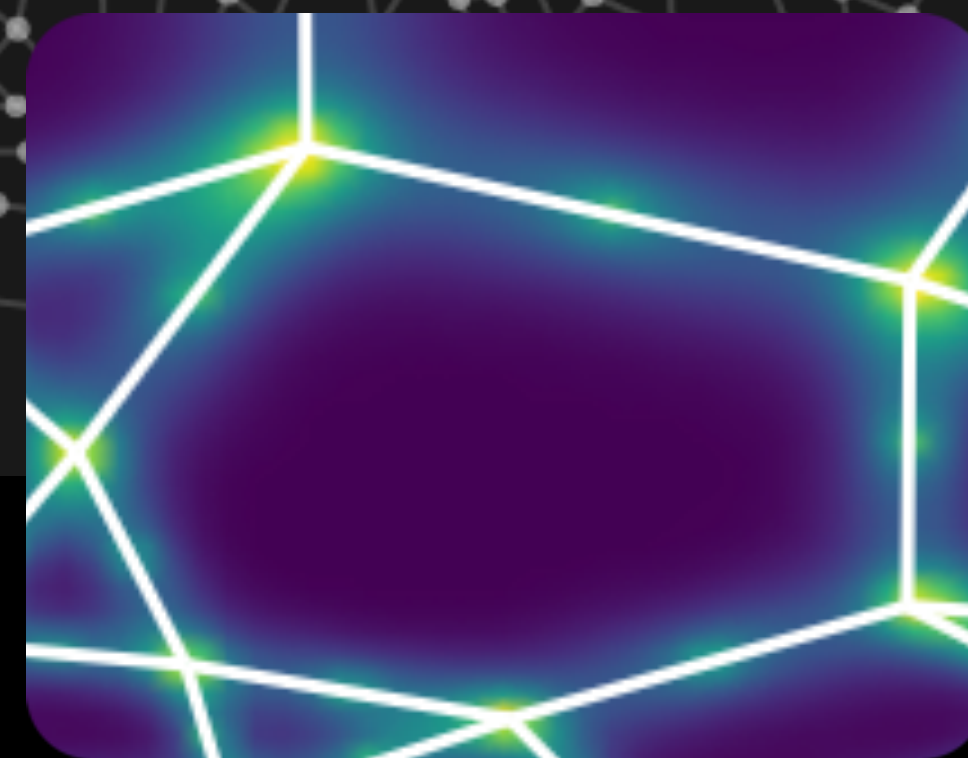
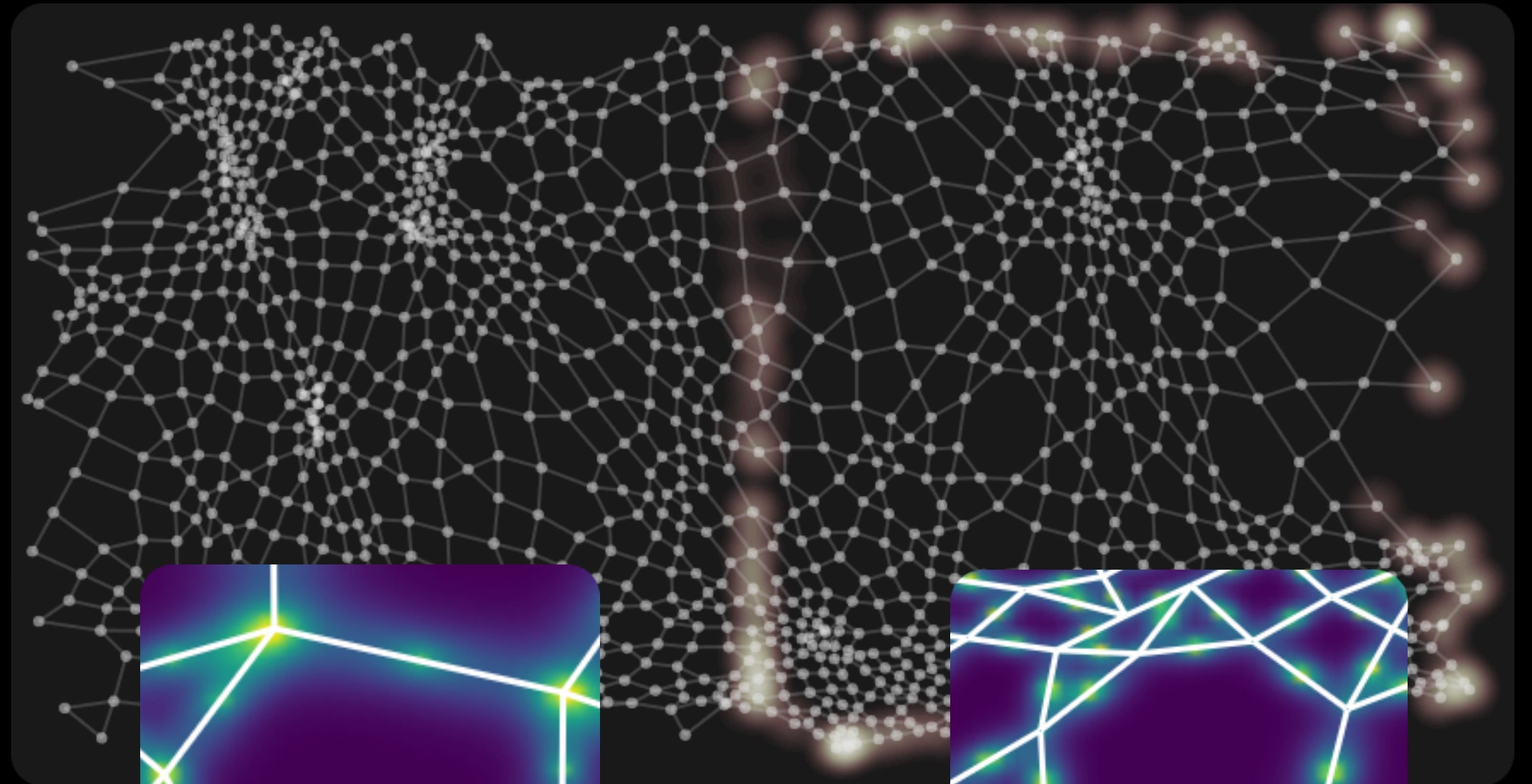
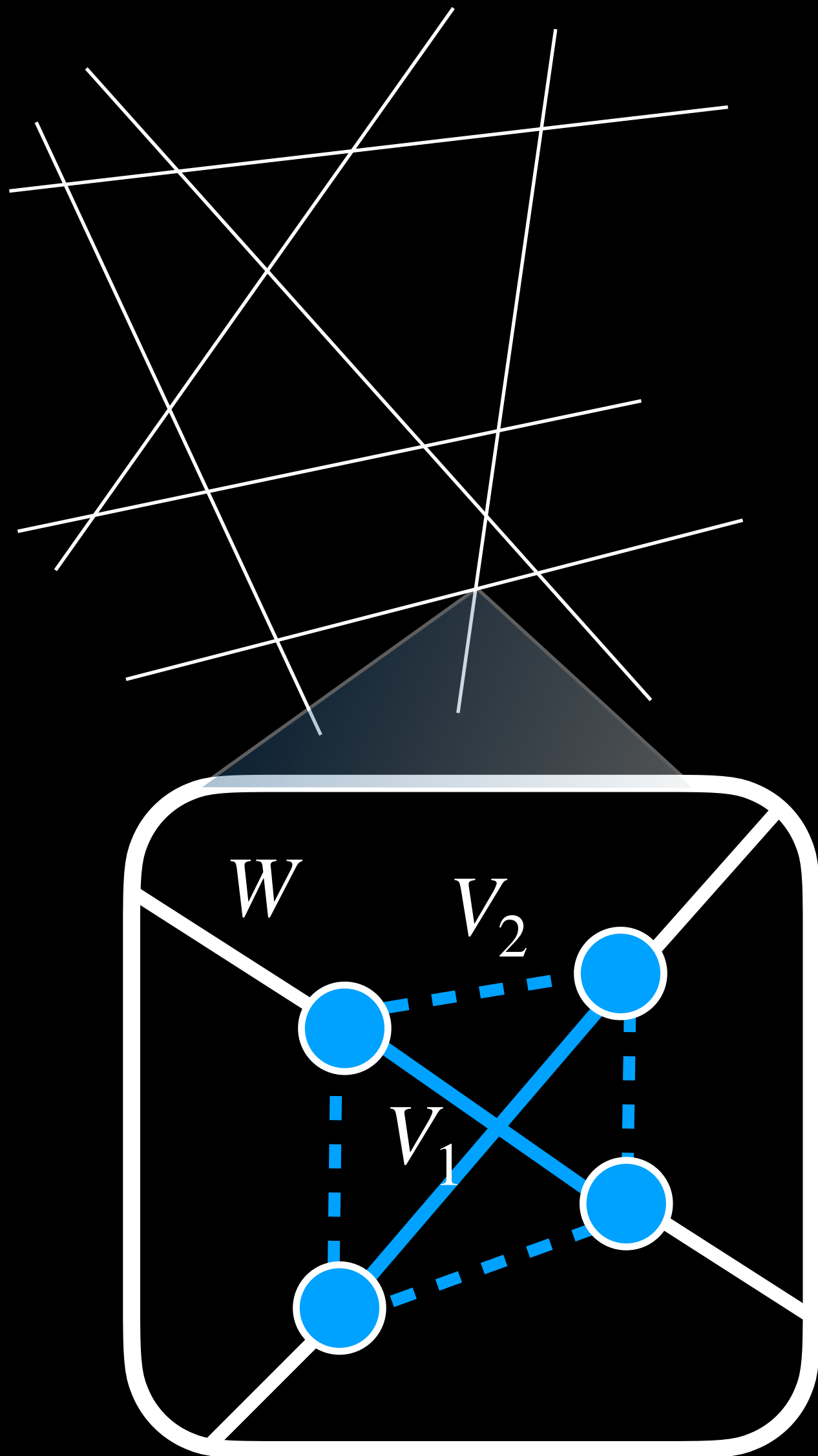


# Mikado model (2D or 3D)

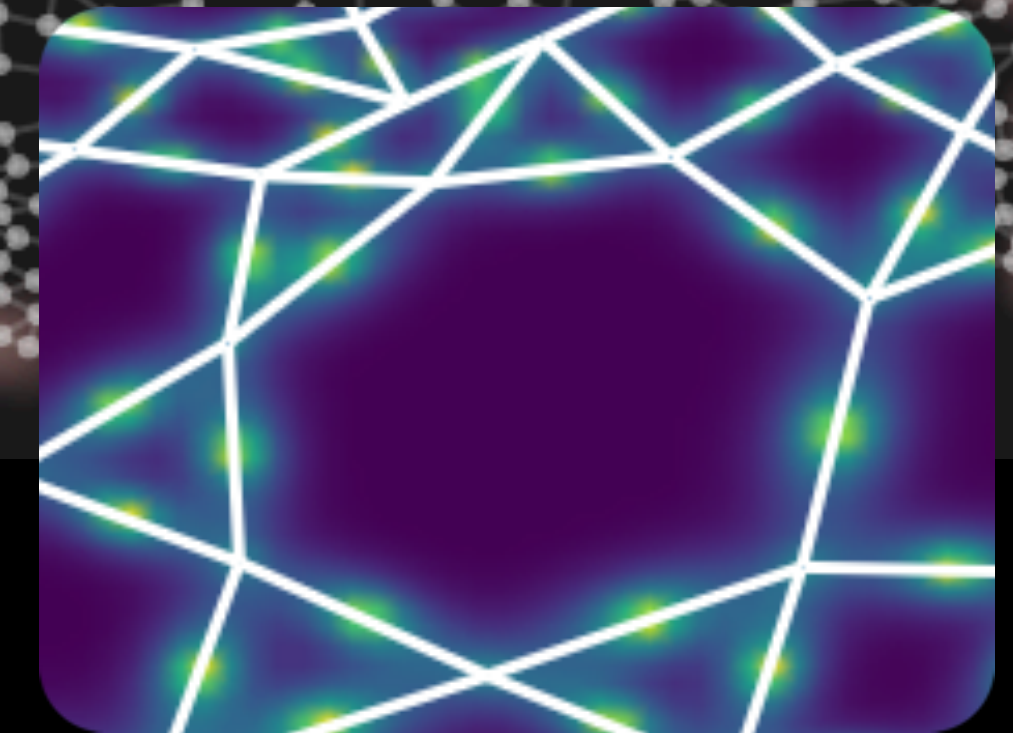
Two obstructed limits

$$W \ll V_{1,2}$$

$$W \gg V_{1,2}$$

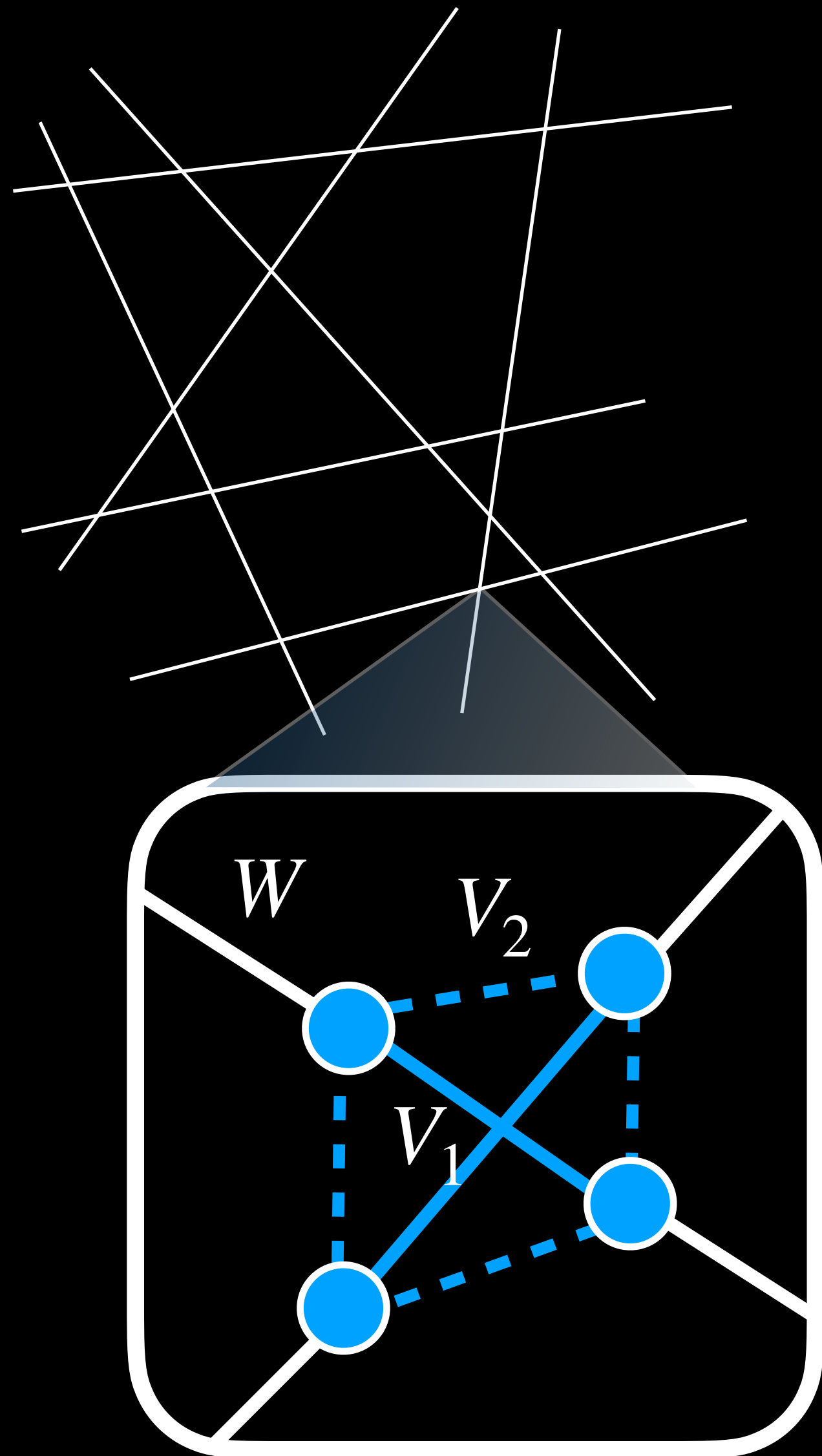


charge on sites



charge on bonds

# Mikado model (2D or 3D)



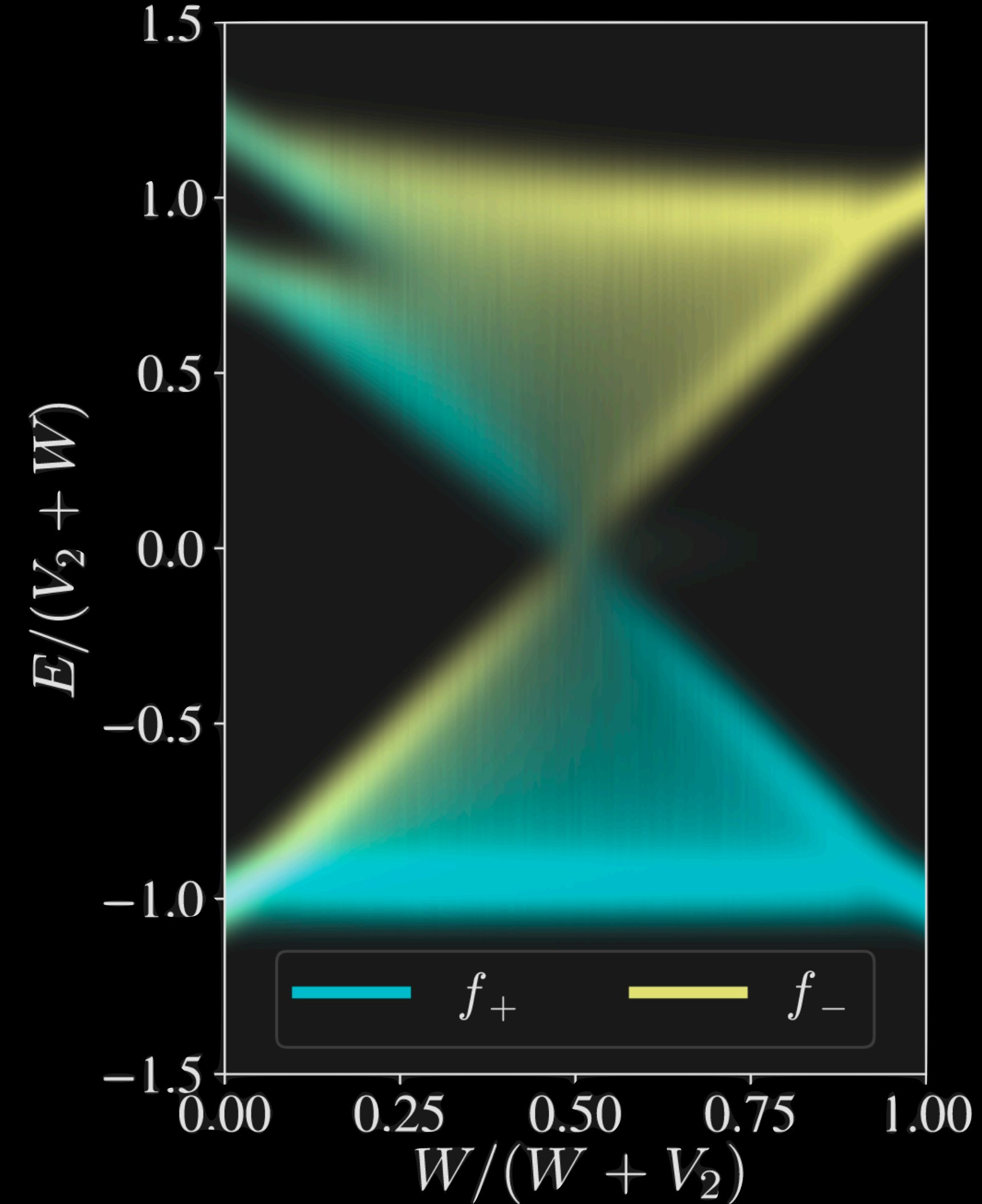
Symmetry indicated

Q. Marsal, D. Varjas, AGG PNAS, (2020)

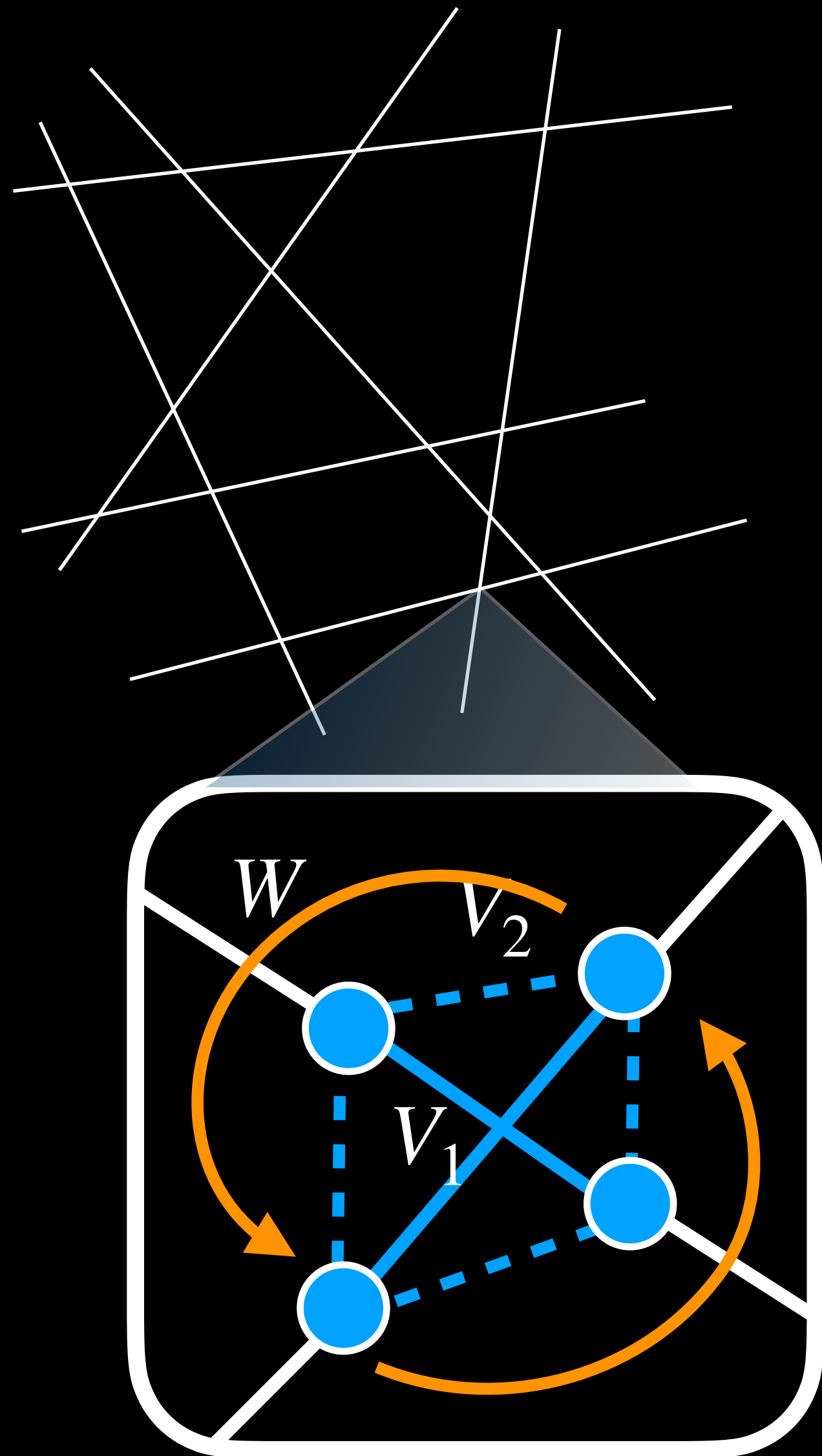
$W \ll V_{1,2}$

$W \gg V_{1,2}$

DOS



# Mikado model (2D or 3D)



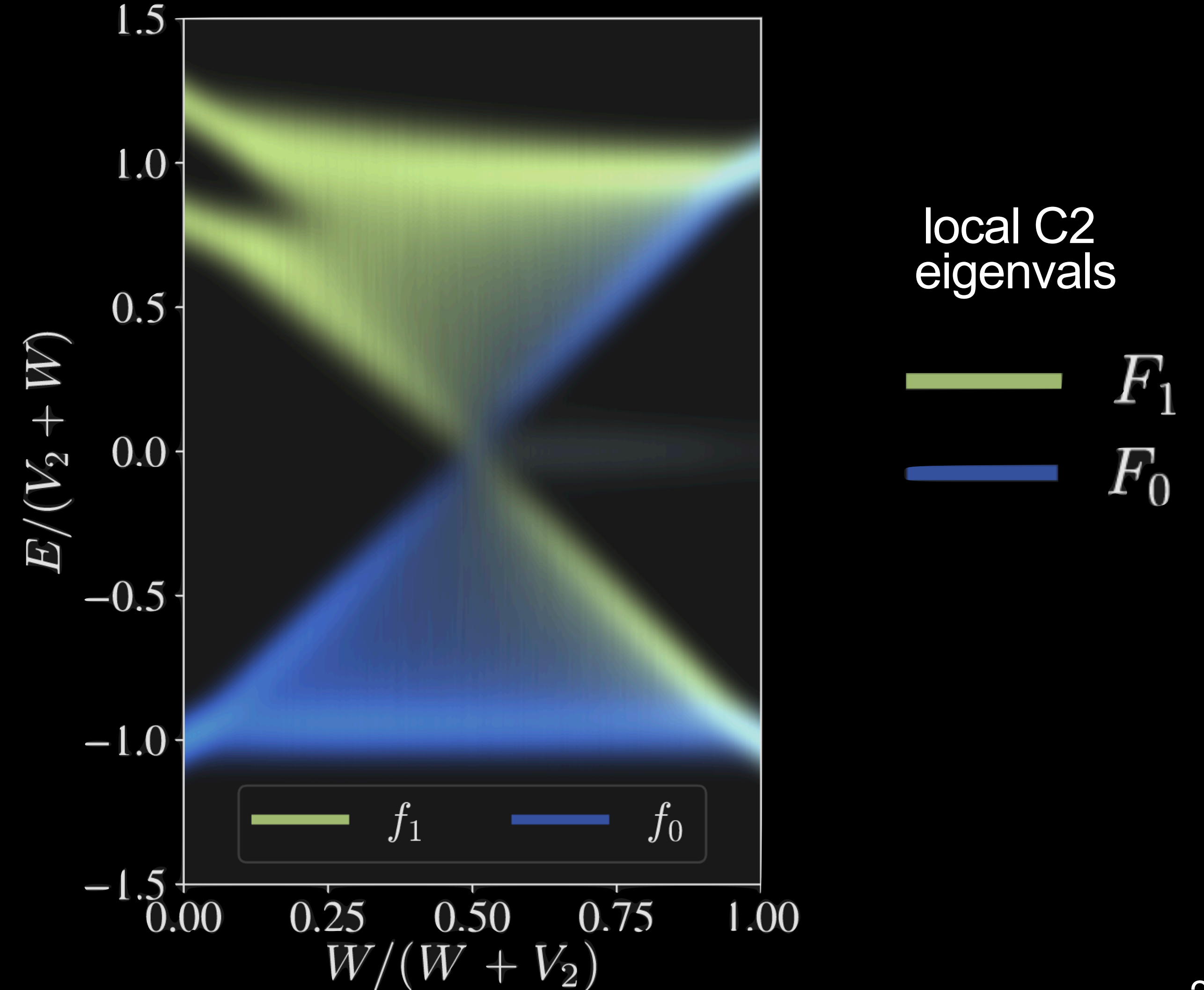
Symmetry indicated

Q. Marsal, D. Varjas, AGG PNAS, (2020)

$W \ll V_{1,2}$

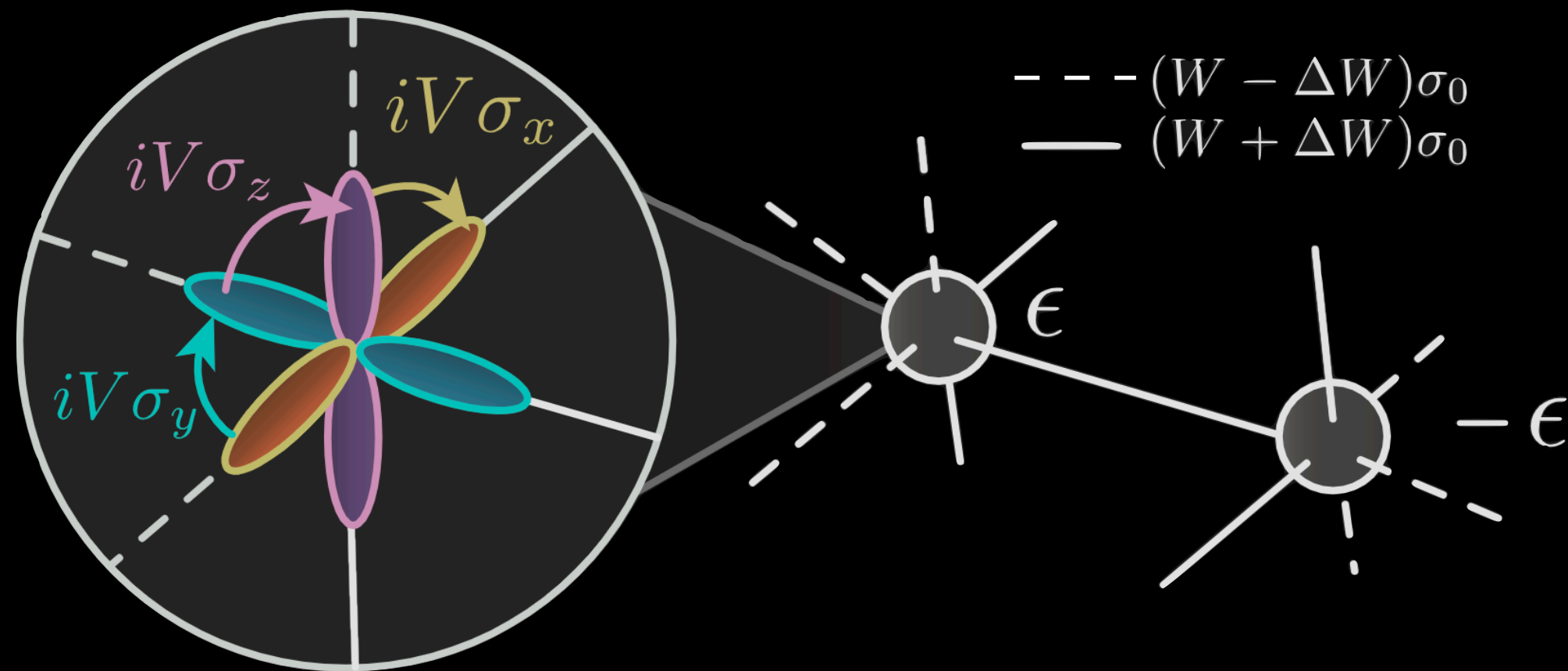
$W \gg V_{1,2}$

DOS



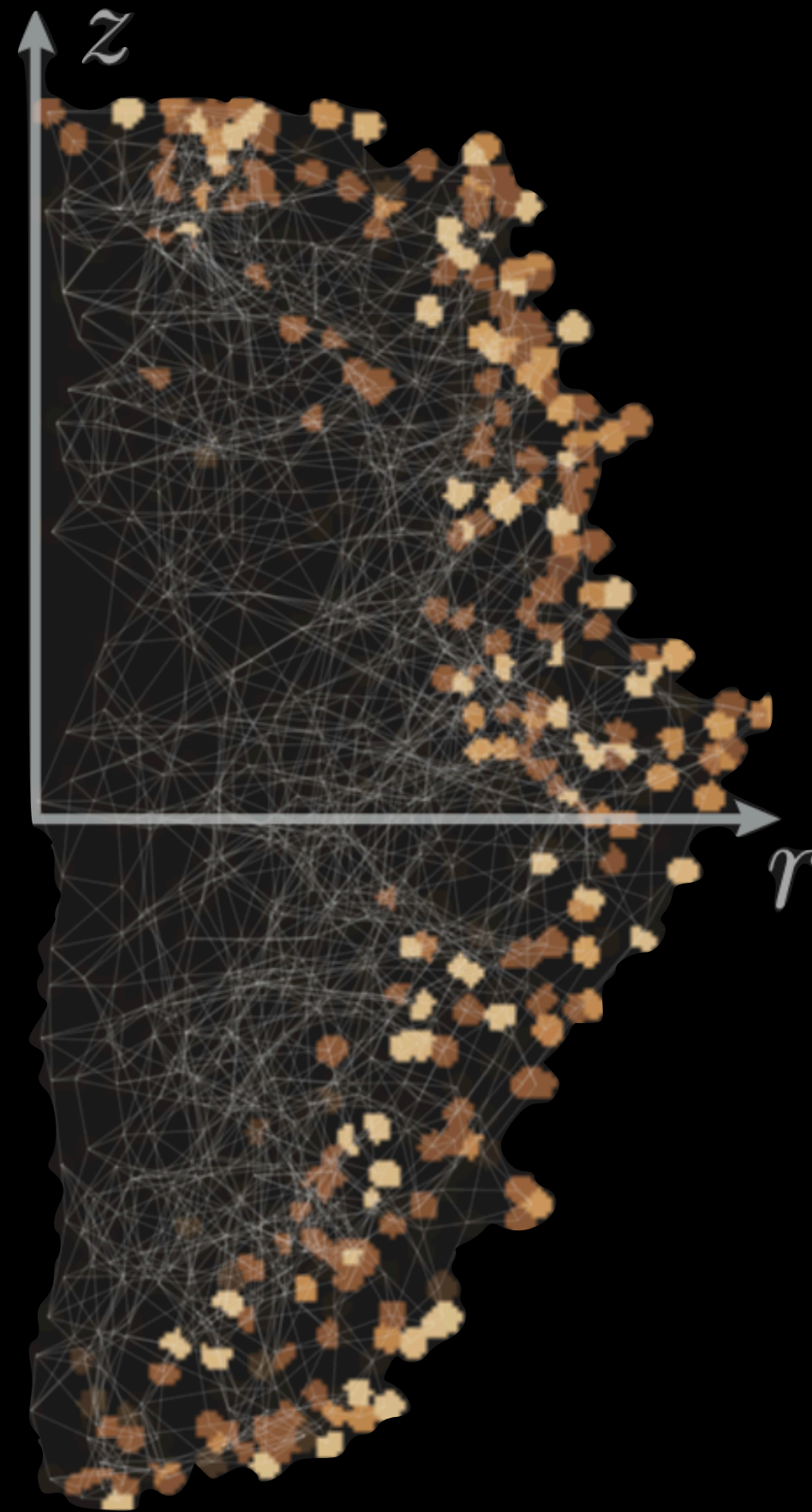
# Phase change material GeTe

## 3-orbital tight-binding model



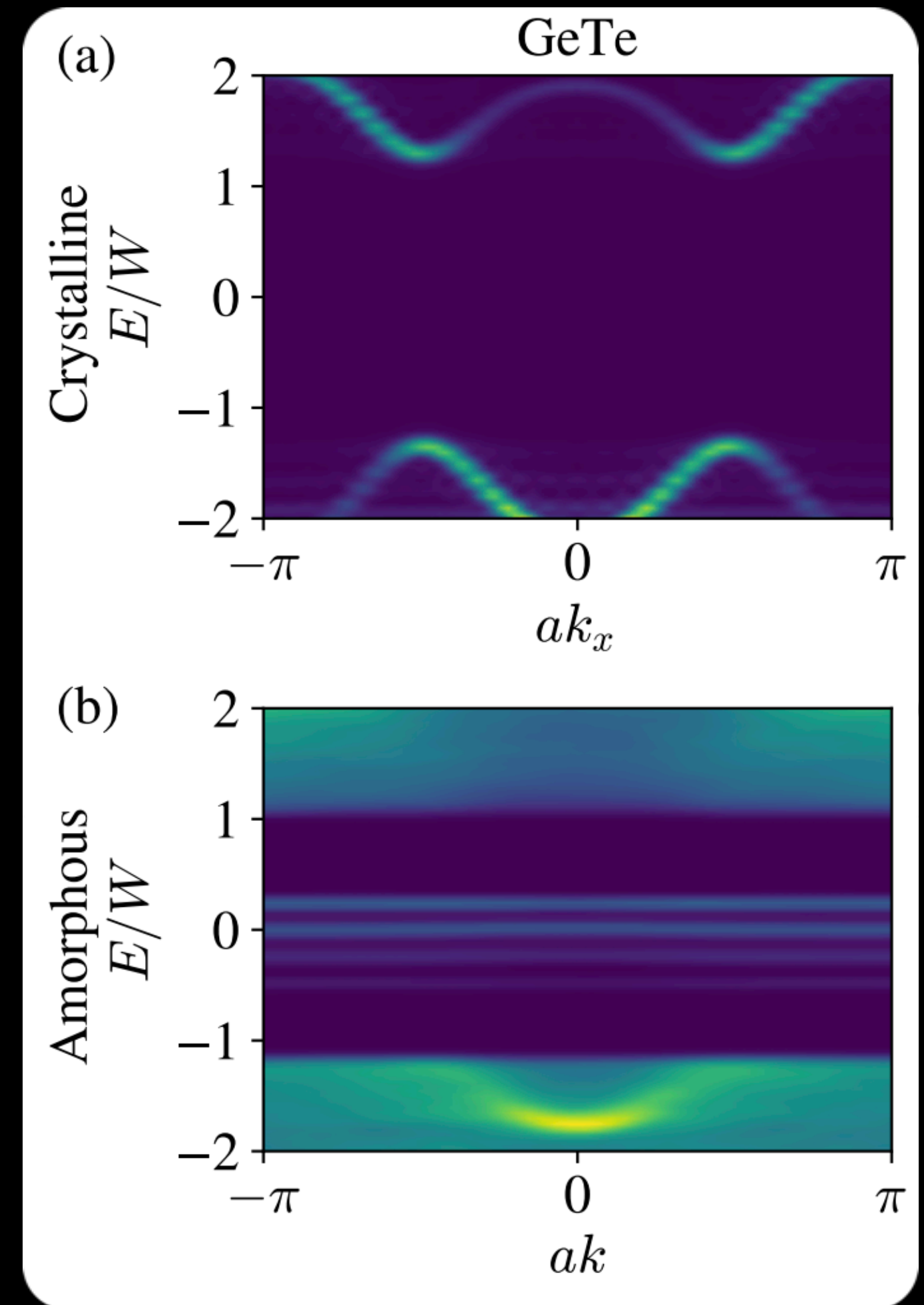
hopping + SOC + onsite energy diff

## in-gap LDOS



2D layer of localized surface states

## ARPES



A flat band switch!

# Predicting amorphous topological solids efficiently?

## Structural spillage

D. Muñoz-Segovia, P. Corbae, F. Hellman, D. Varjas, S. Griffin, AGG, arXiv: 2301.02686



Daniel  
Muñoz-Segovia

DIPC



Paul  
Corbae

Berkeley



Frances  
Hellmann

Berkeley



Daniel  
Varjas

MPI Dresden



Sinead  
Griffin

LBNL Berkeley

# Predicting amorphous topological solids efficiently?



compare crystal — known topology

with amorphous — unknown topology



Daniel  
Muñoz-Segovia

DIPC



Paul  
Corbae

Berkeley



Frances  
Hellmann

Berkeley



Daniel  
Varjas

MPI Dresden



Sinead  
Griffin

LBNL Berkeley

# Spillage

$P$	topo	high	low
	trivial	low	high
		trivial	topo
		$\tilde{P}$	

$$P = \sum_{n \in \text{occ}} |\psi_n\rangle \langle \psi_n|$$

$$\gamma = \text{Tr}[(P - \tilde{P})^2] / 2$$

↑
↑  
 Test system (unknown)      Reference system (known)

**spin-orbit spillage**

Liu and Vanderbilt PRB (2014)

with spin-orbit

vs without spin-orbit

**structural spillage**

amorphous

vs

crystalline



# Spillage

$P$	topo	high	low
	trivial	low	high
		trivial	topo
		$\tilde{P}$	

$$P = \sum_{n \in \text{occ}} |\psi_n\rangle \langle \psi_n|$$

$$\gamma = \text{Tr}[(P - \tilde{P})^2] / 2$$

↑
↑  
 Test system (unknown)      Reference system (known)

\*k and G are well defined

# Momentum resolved

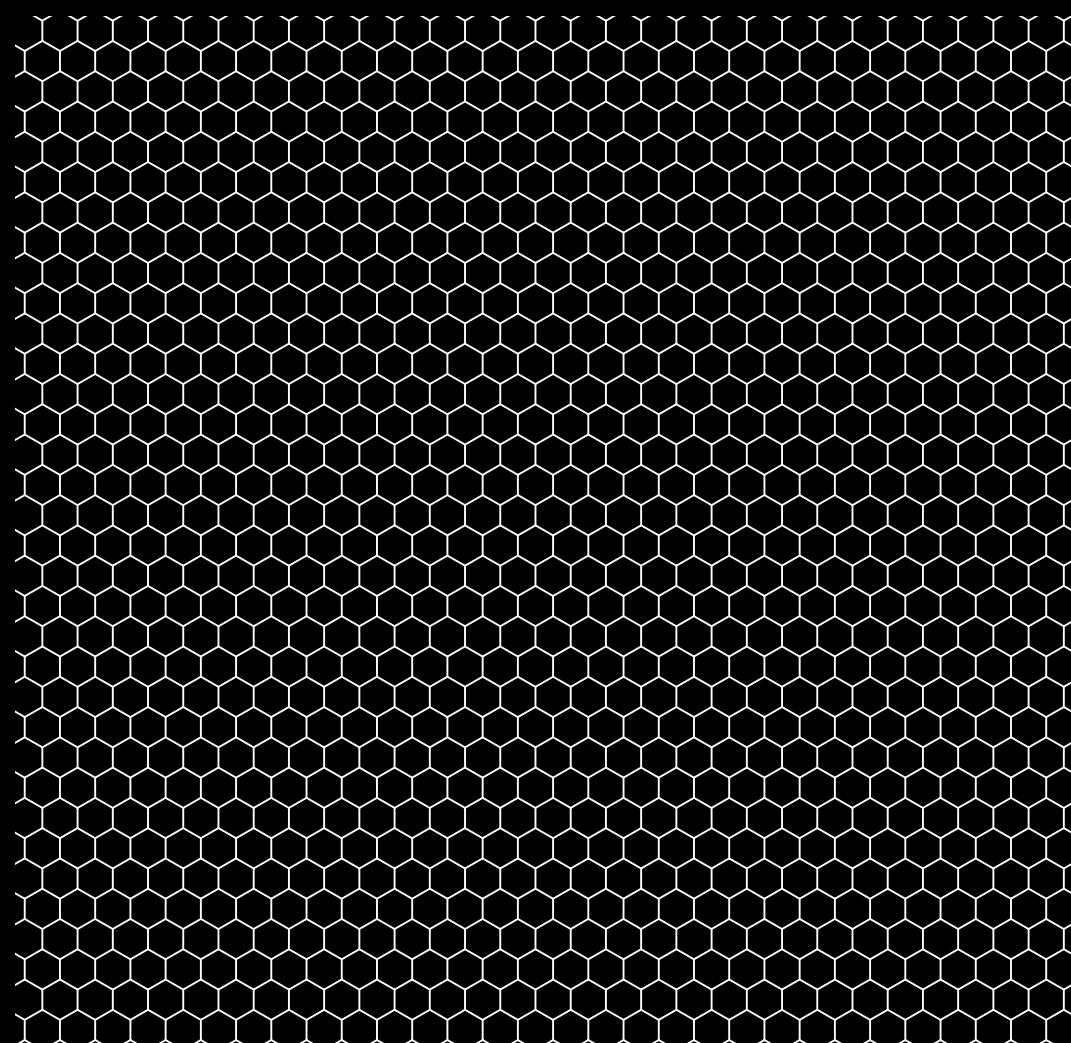
$$\gamma_{\text{qB}}(\mathbf{k}) = \frac{1}{2} \left\{ \left[ \sum_{G\alpha} P_{k+G, k+G}^{\alpha\alpha} \right] + \tilde{n}_{\text{occ}}(\mathbf{k}) - \sum_{G\alpha} \sum_{G'\beta} \left[ P_{k+G, k+G'}^{\alpha\beta} \tilde{P}_{k+G', k+G}^{\beta\alpha} + \tilde{P}_{k+G, k+G'}^{\alpha\beta} P_{k+G', k+G}^{\beta\alpha} \right] \right\}$$

structural spillage

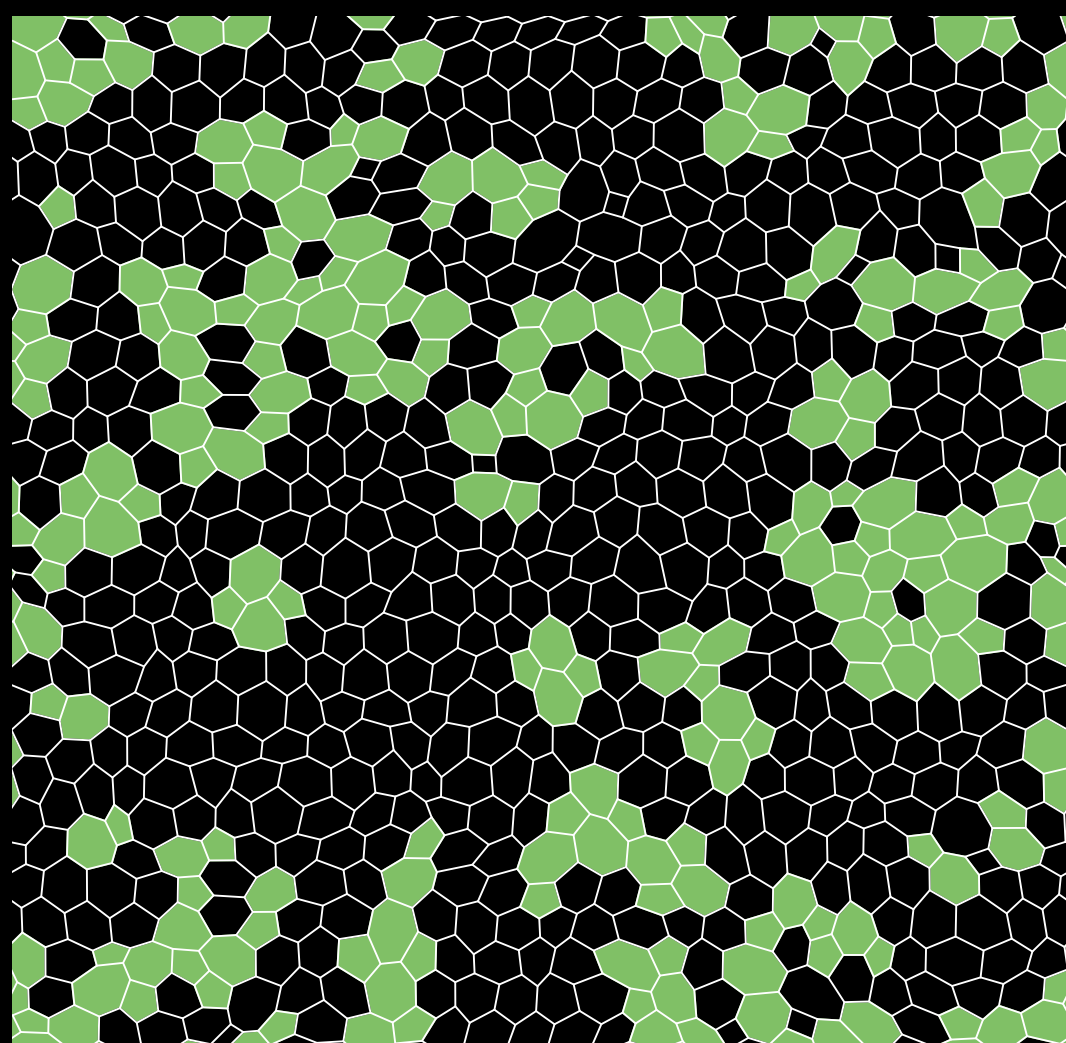
amorphous vs crystalline

# A new knob

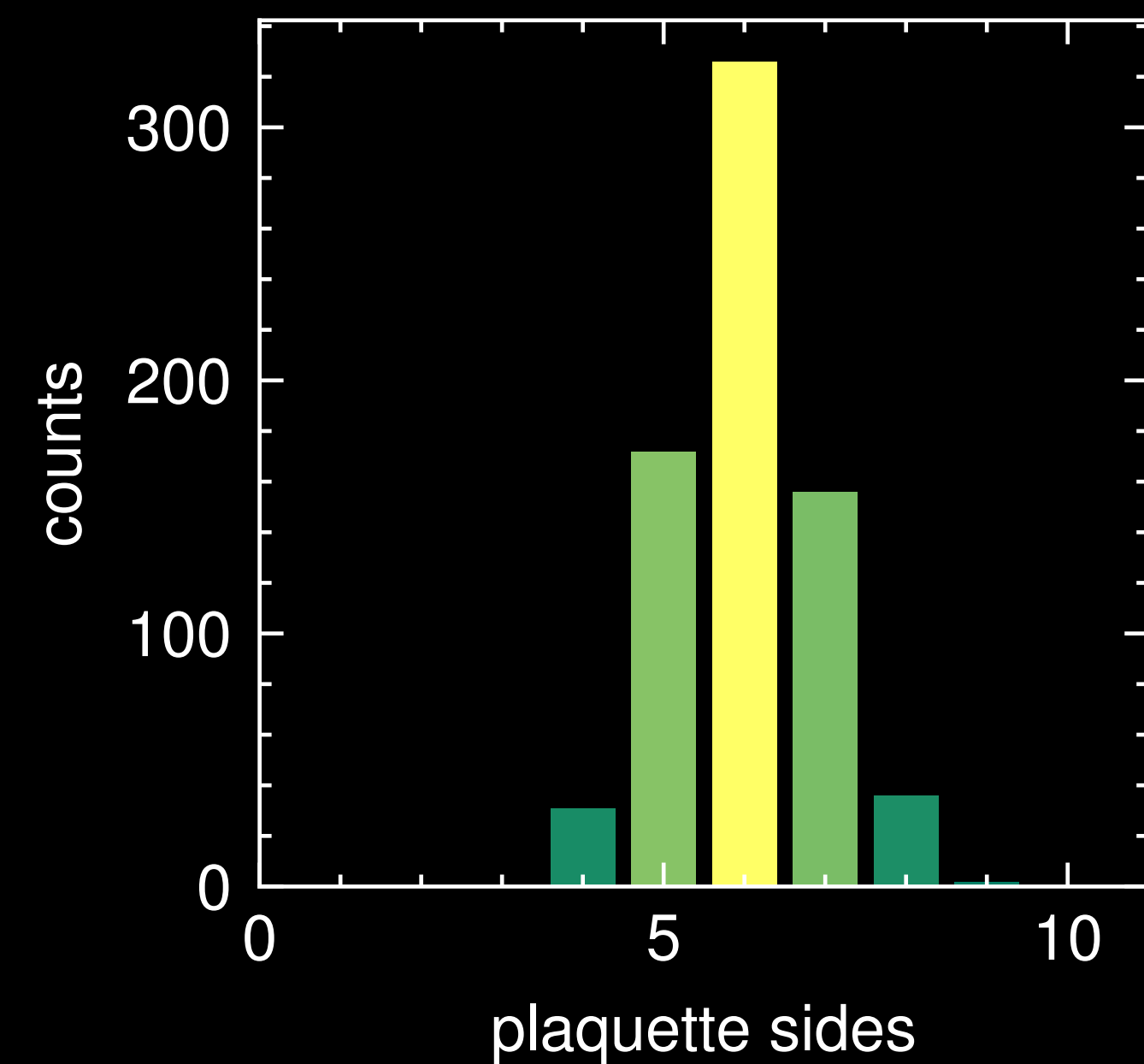
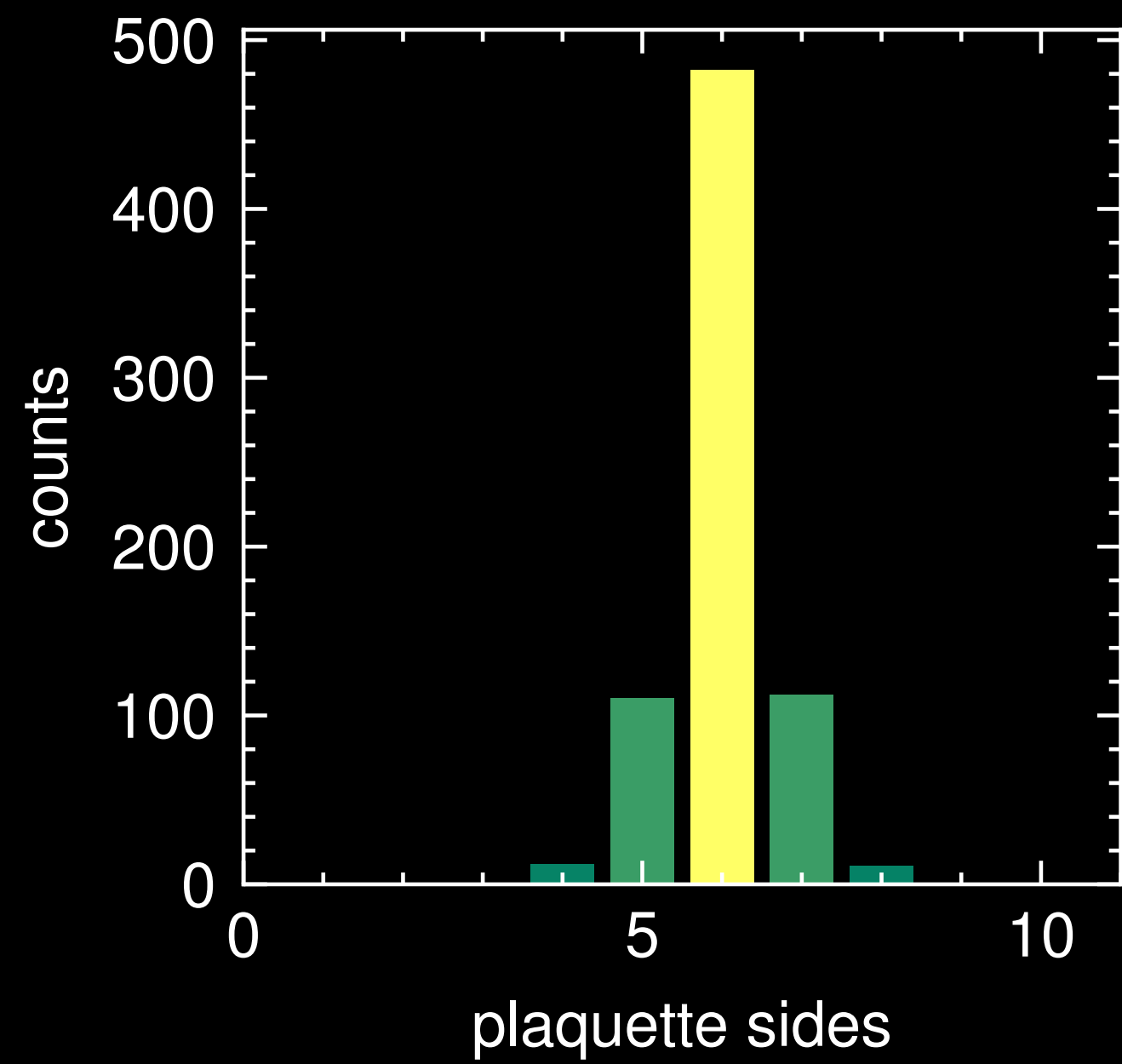
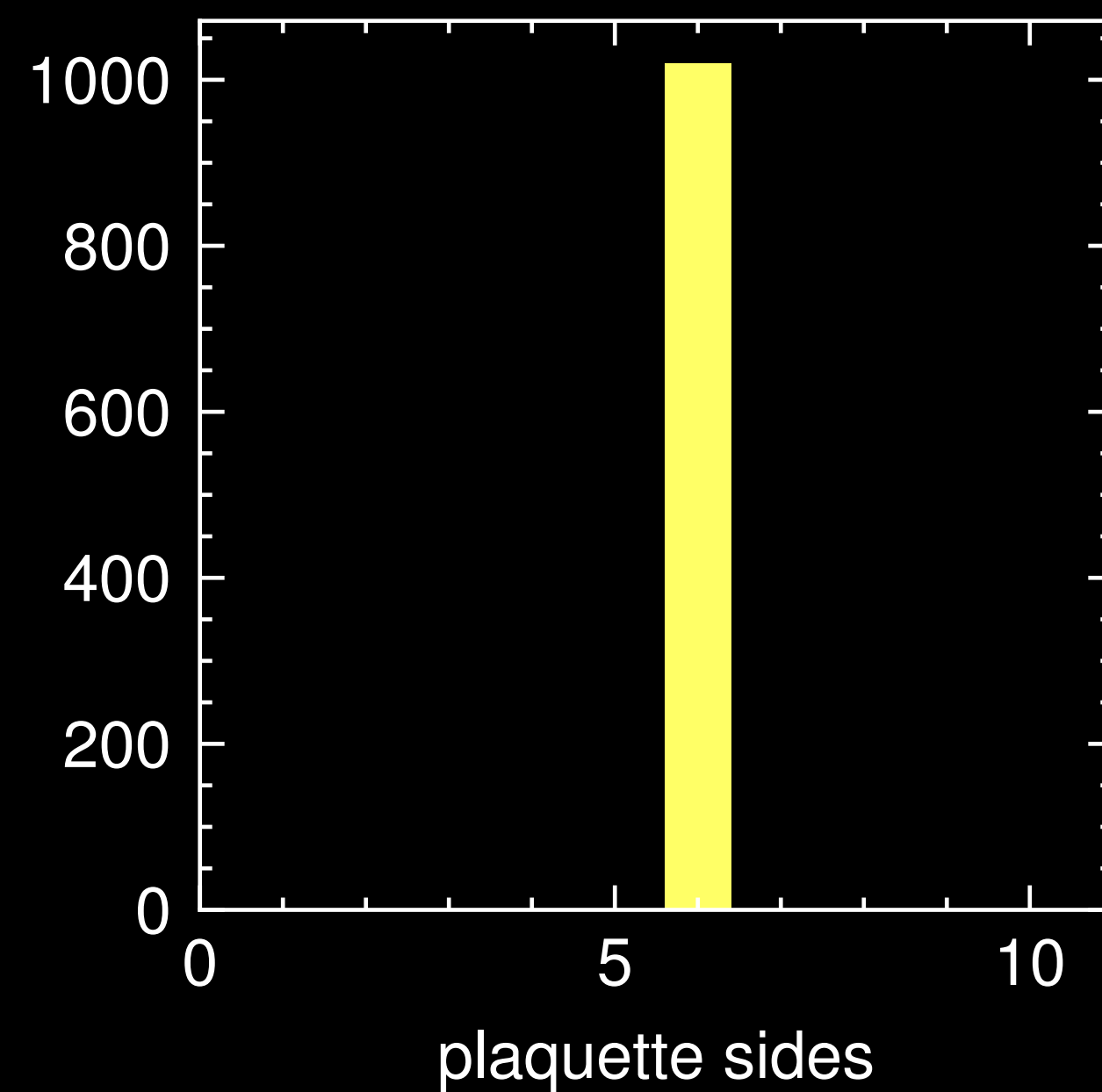
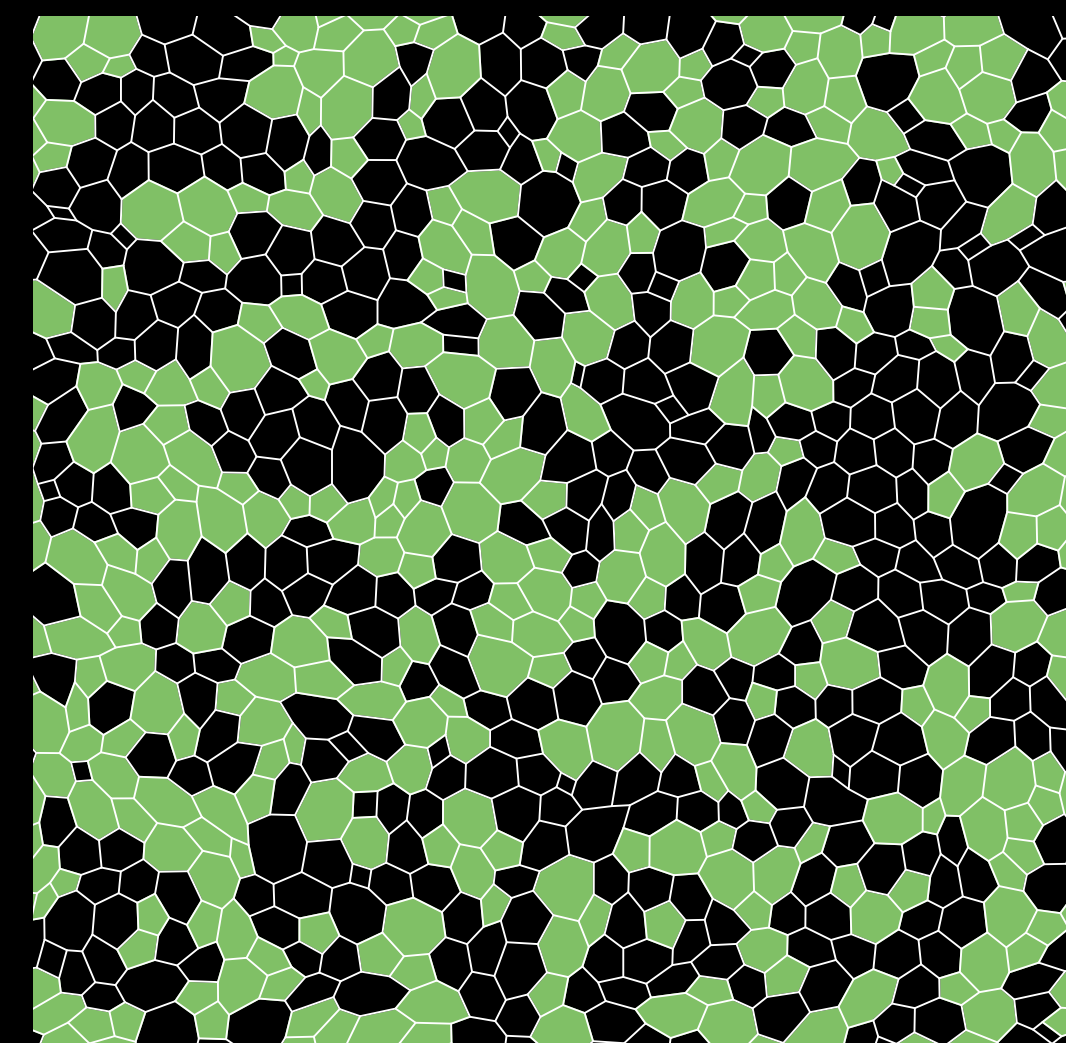
crystal



polycrystal



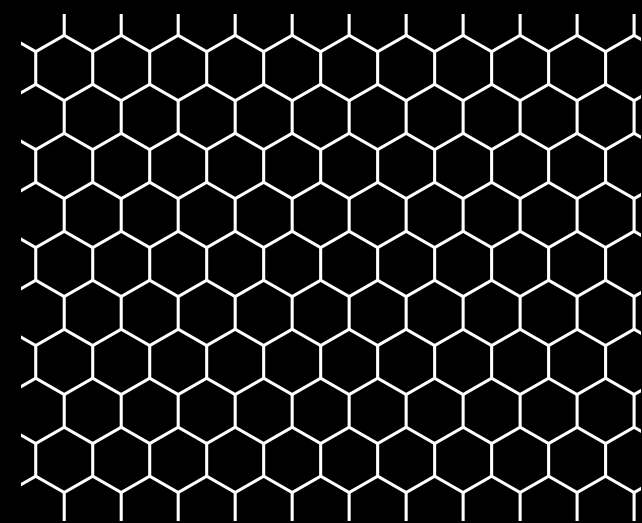
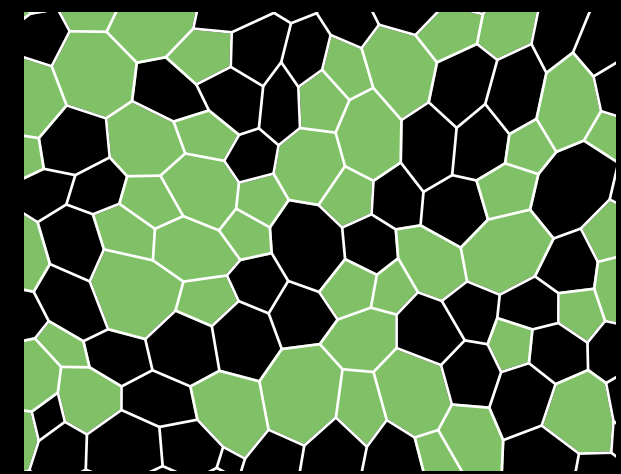
amorphous



# Tight-binding benchmark

## Amorphous Bismuthene

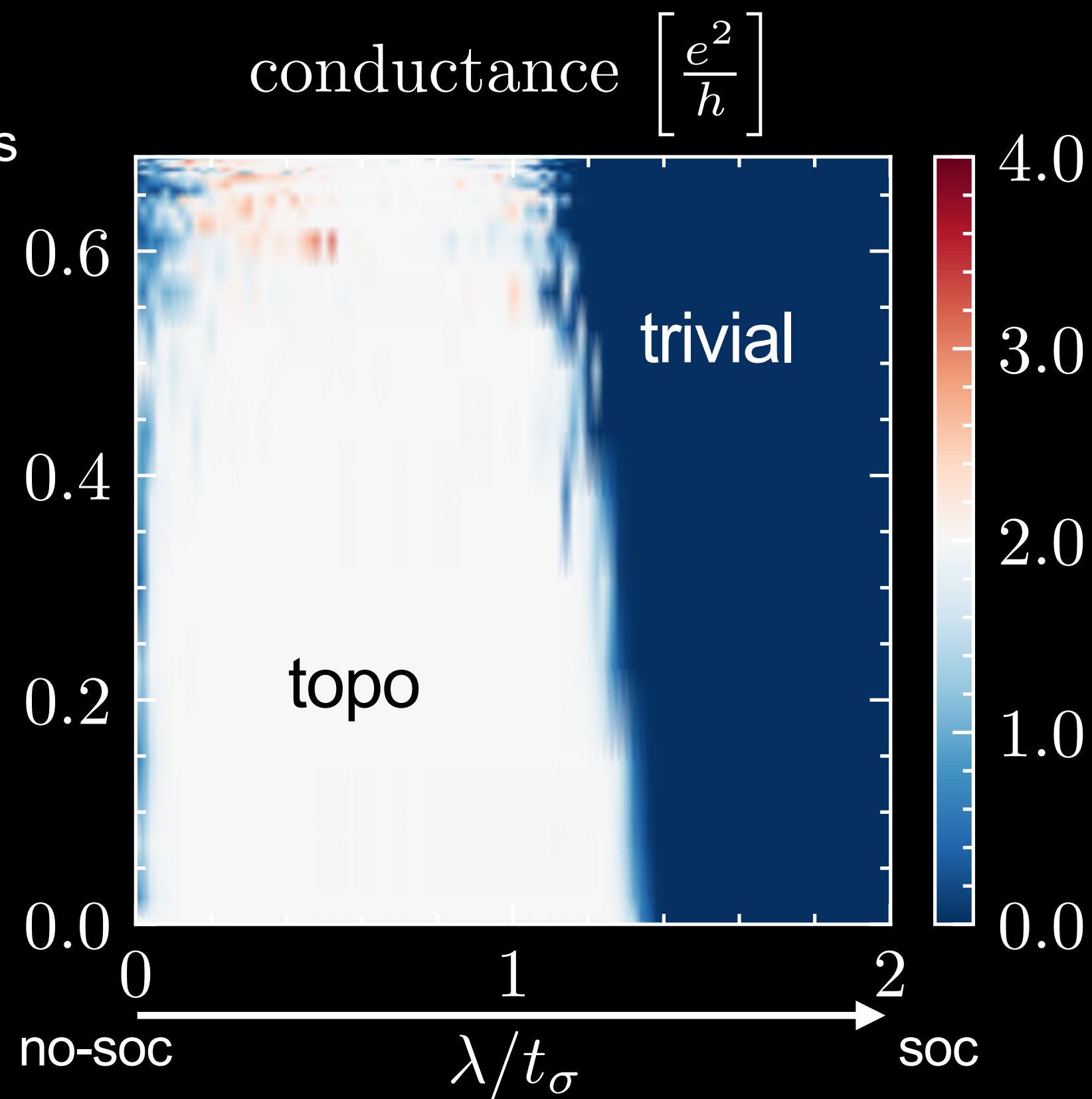
Costa, et al Nano Letters (2019)  
Focasio et al 2D Materials (2021)



↑ amorphous

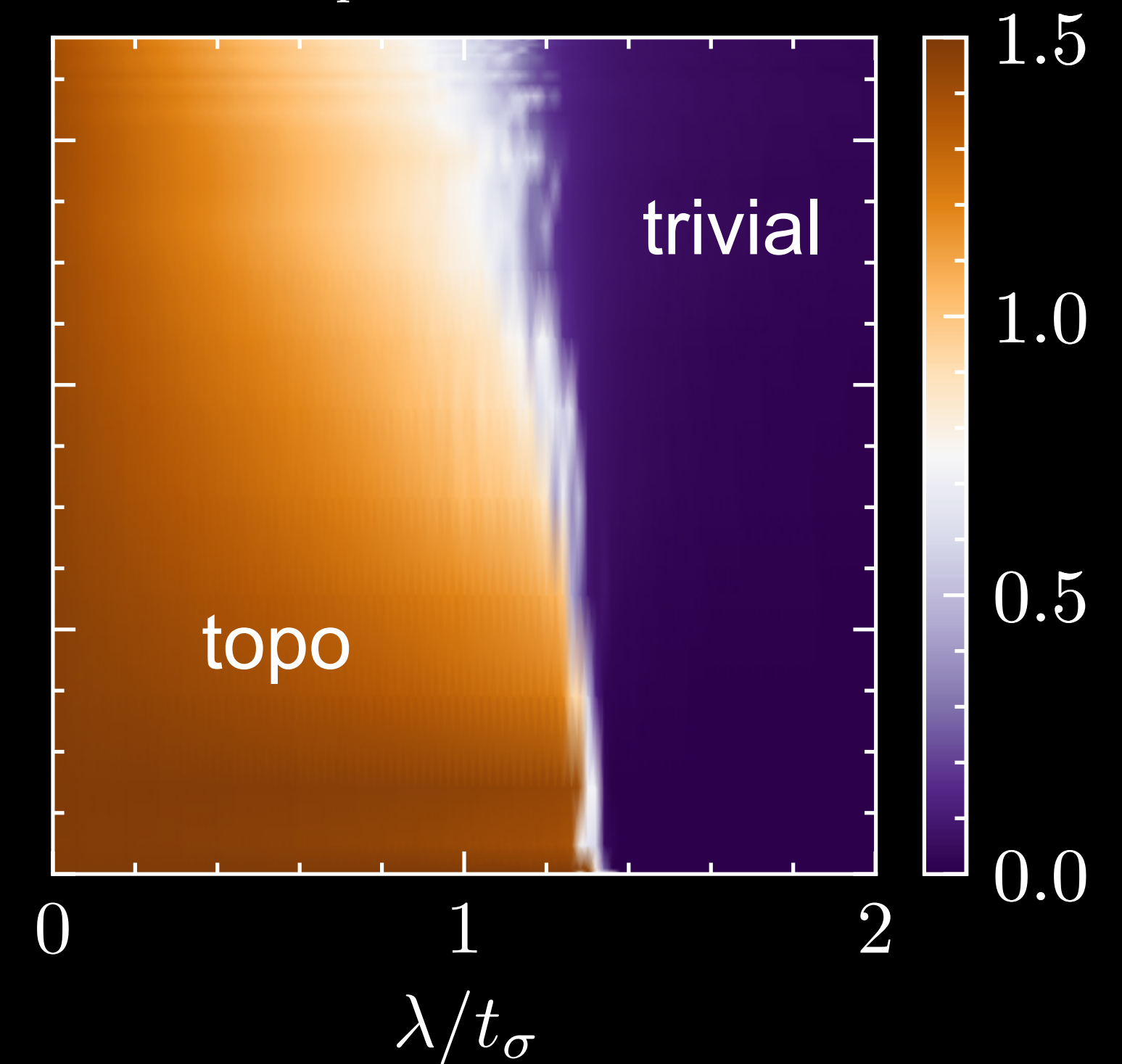
↓ crystal

$\rho_{\text{non-hex}}$



structural spillage

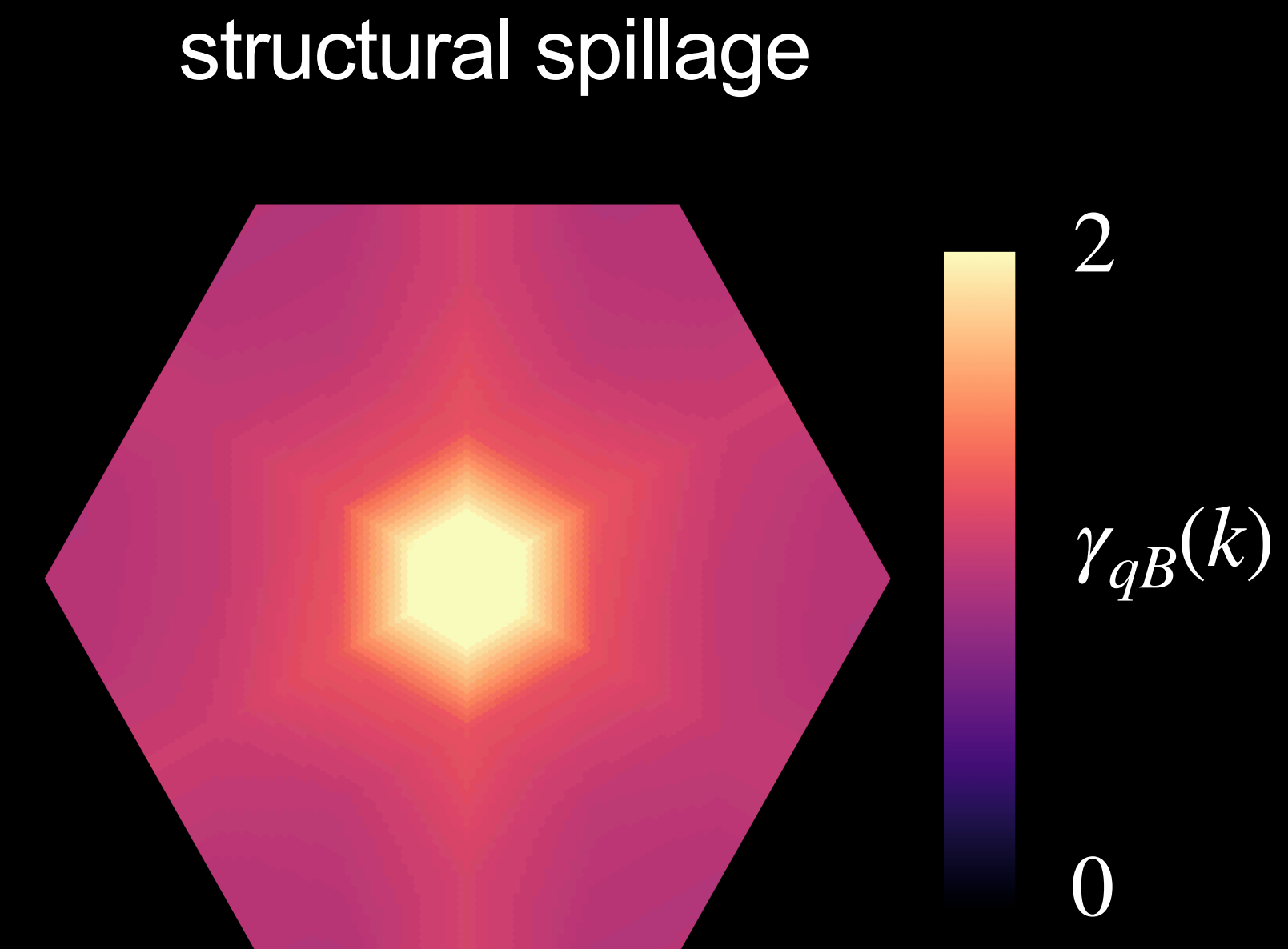
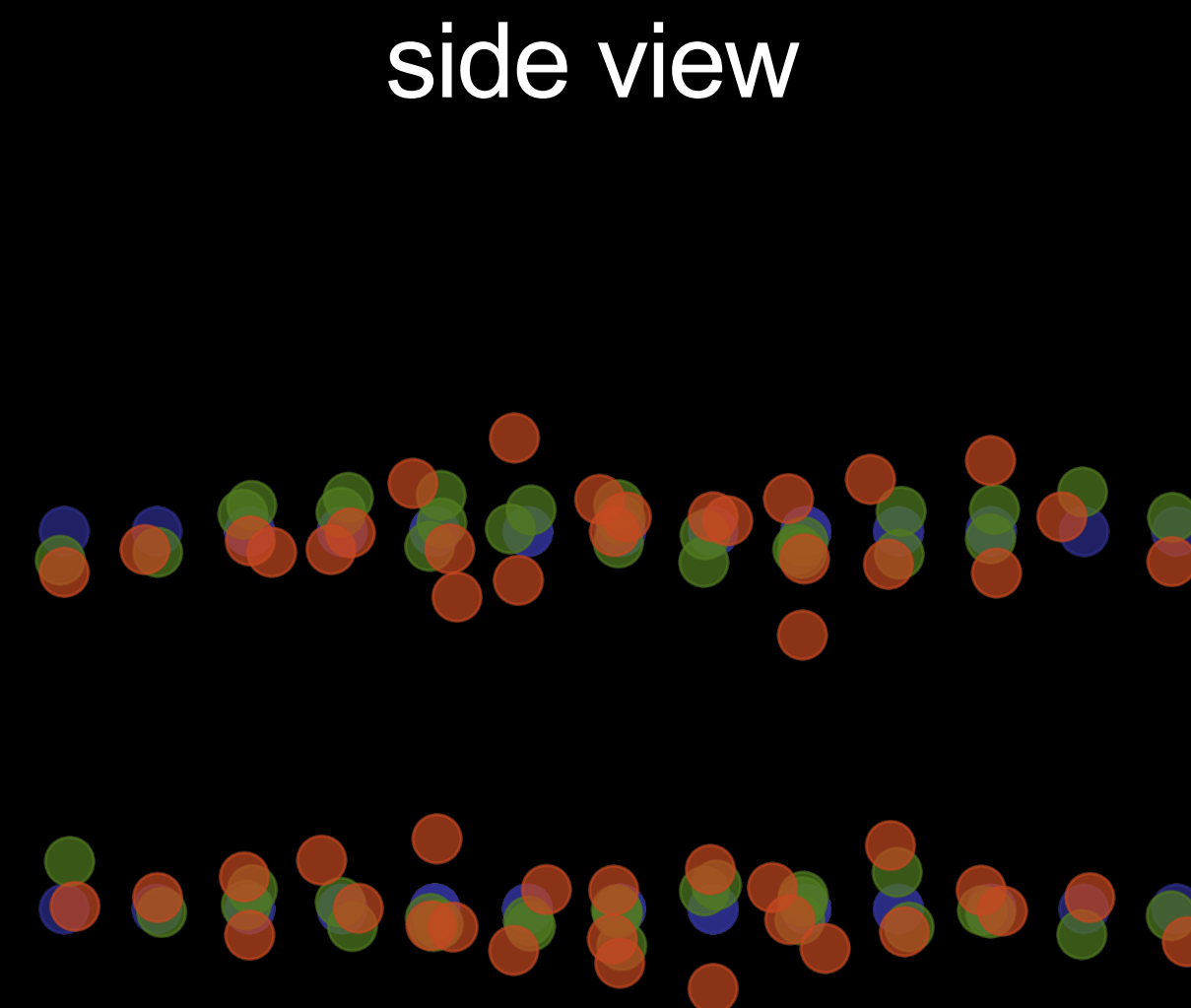
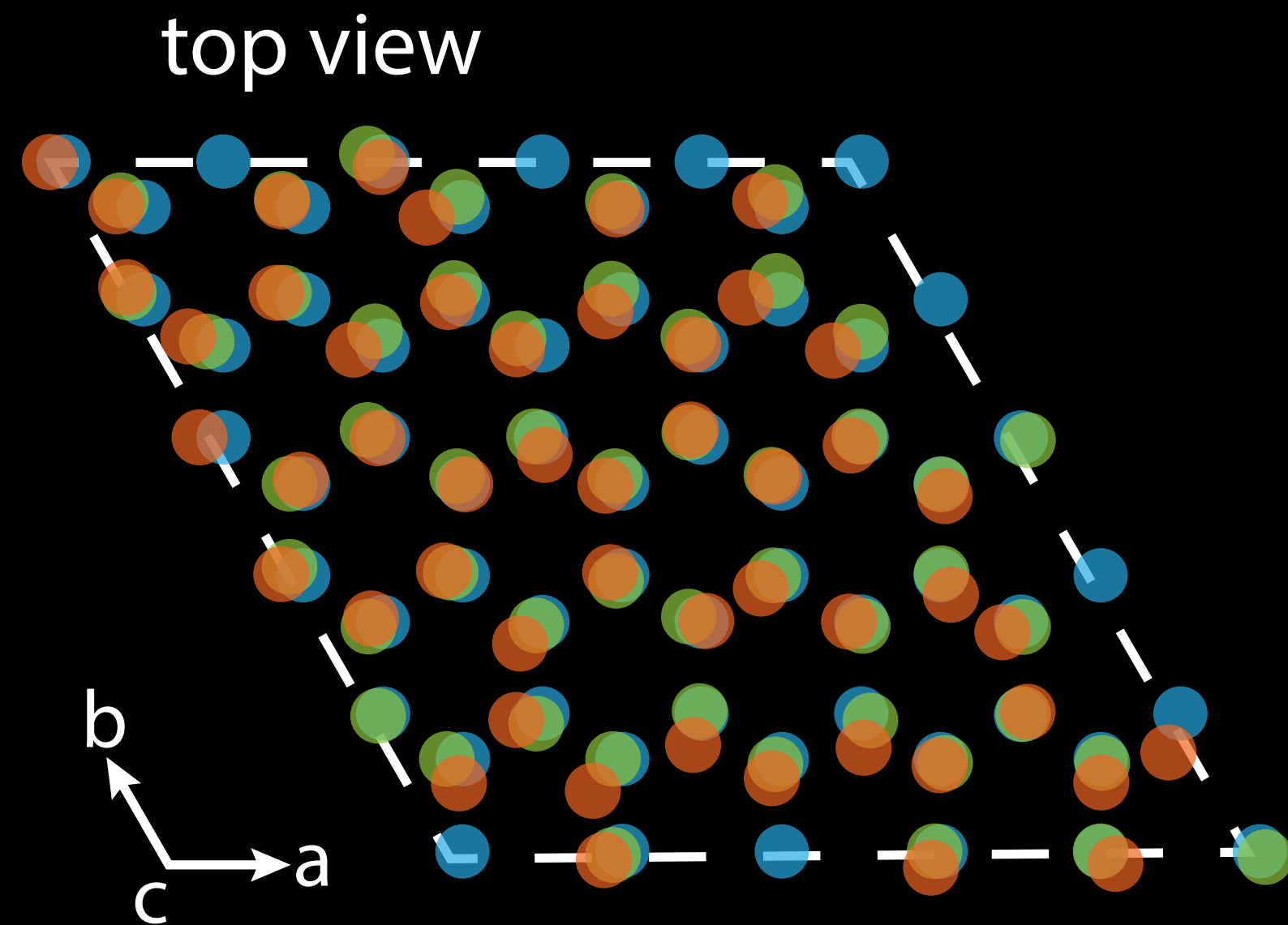
$$\gamma_{\text{qB}}^{\text{TB}}(k=0)$$



# DFT benchmark

amorphous Bismuth bilayer

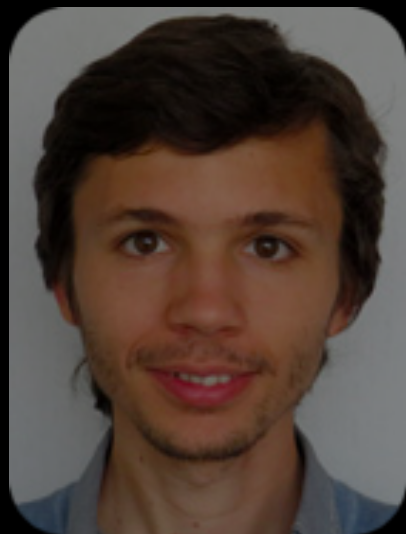
DFT compatible = high-throughput search!



## What's new?

### Flat-band switch

Q. Marsal, D. Varjas, *AGG Phys Rev B*, (2020)



Quentin Marsal  
Néel Institute



Daniel Varjas  
MPI PKS

### Amorphous chiral spin-liquid

AGG, C. Repellin 2210.13548

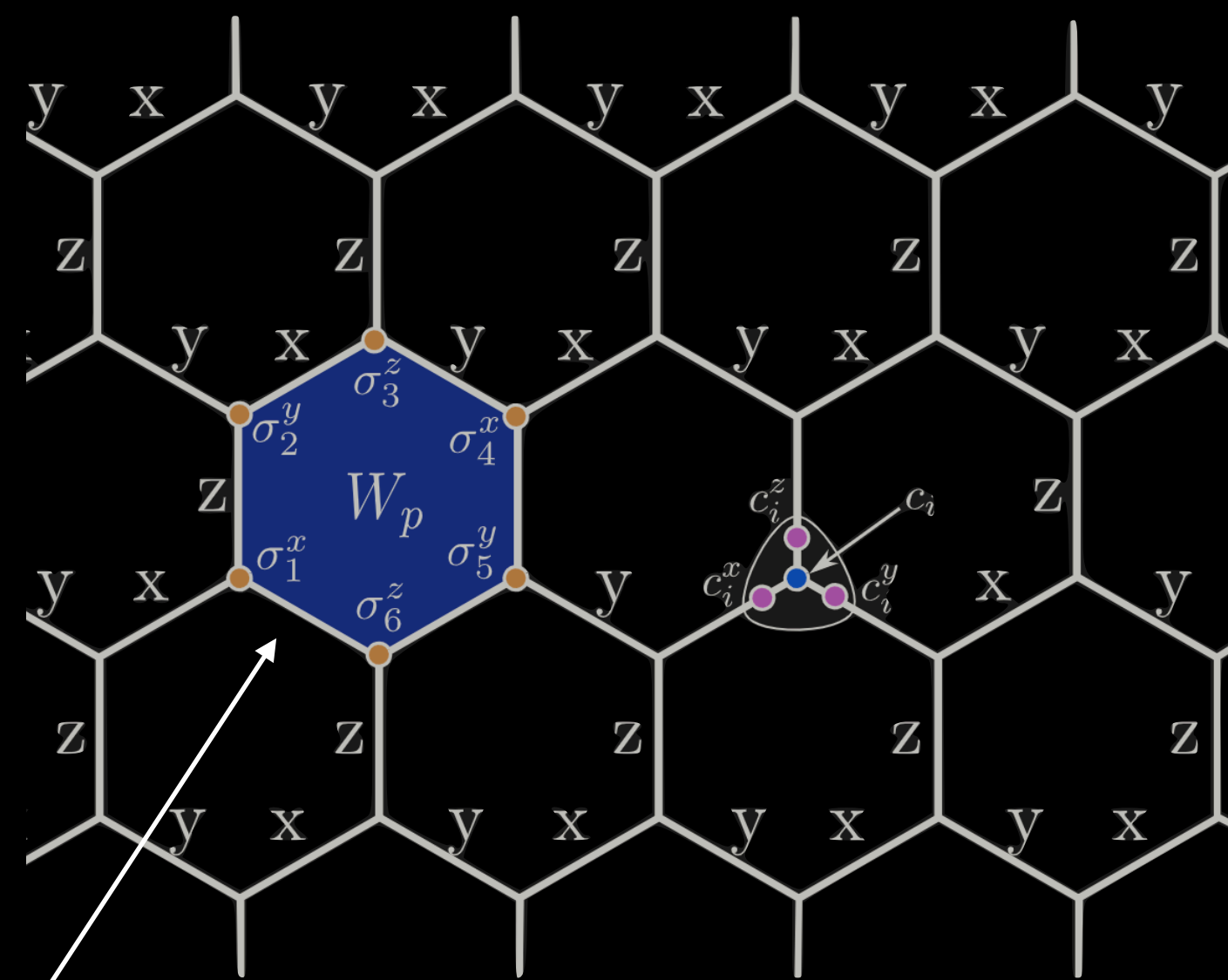


Cécile Repellin  
LPMMC / Grenoble

# Kitaev models

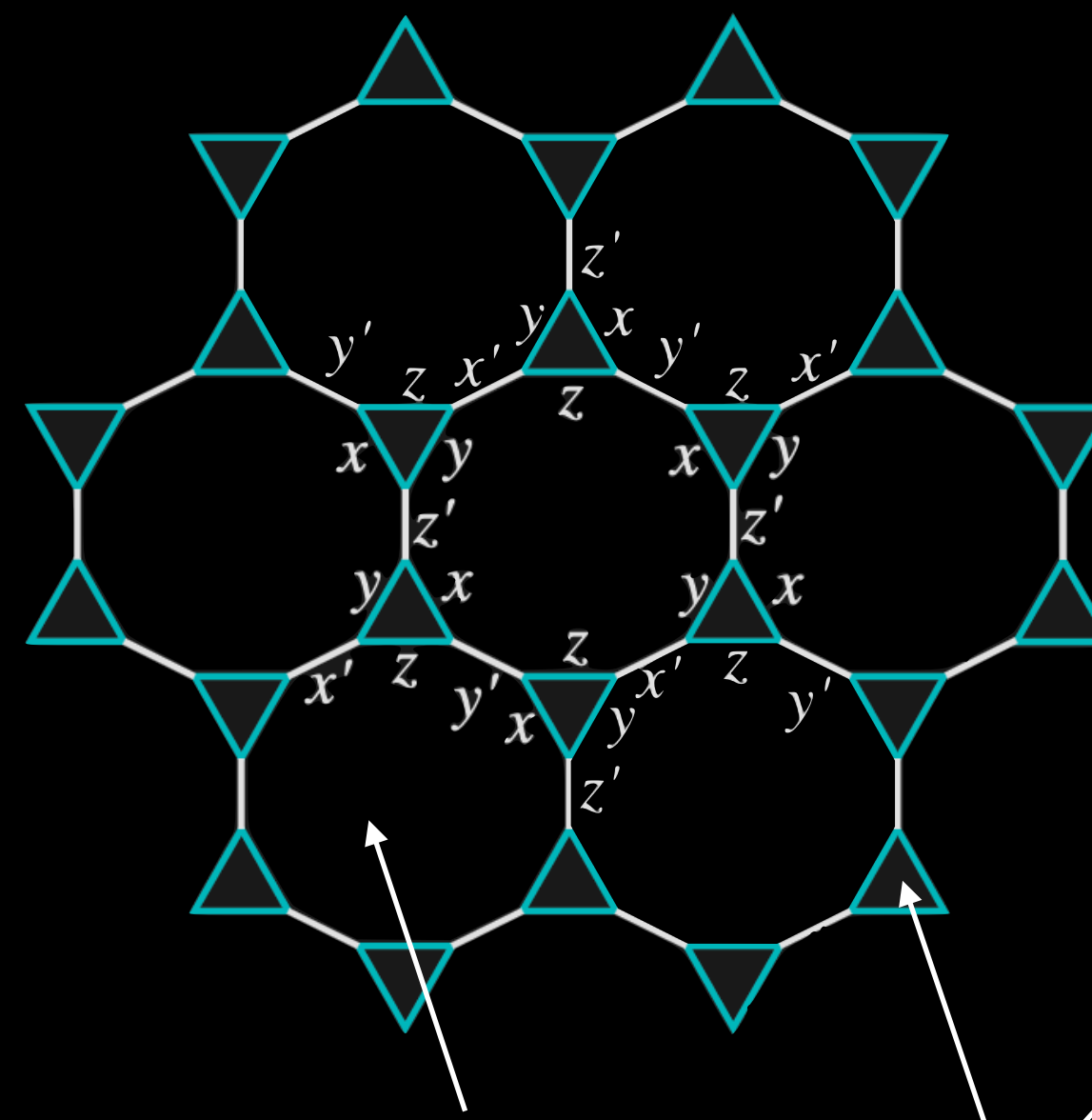
## Honeycomb

Kitaev Ann. Phys. (2006)



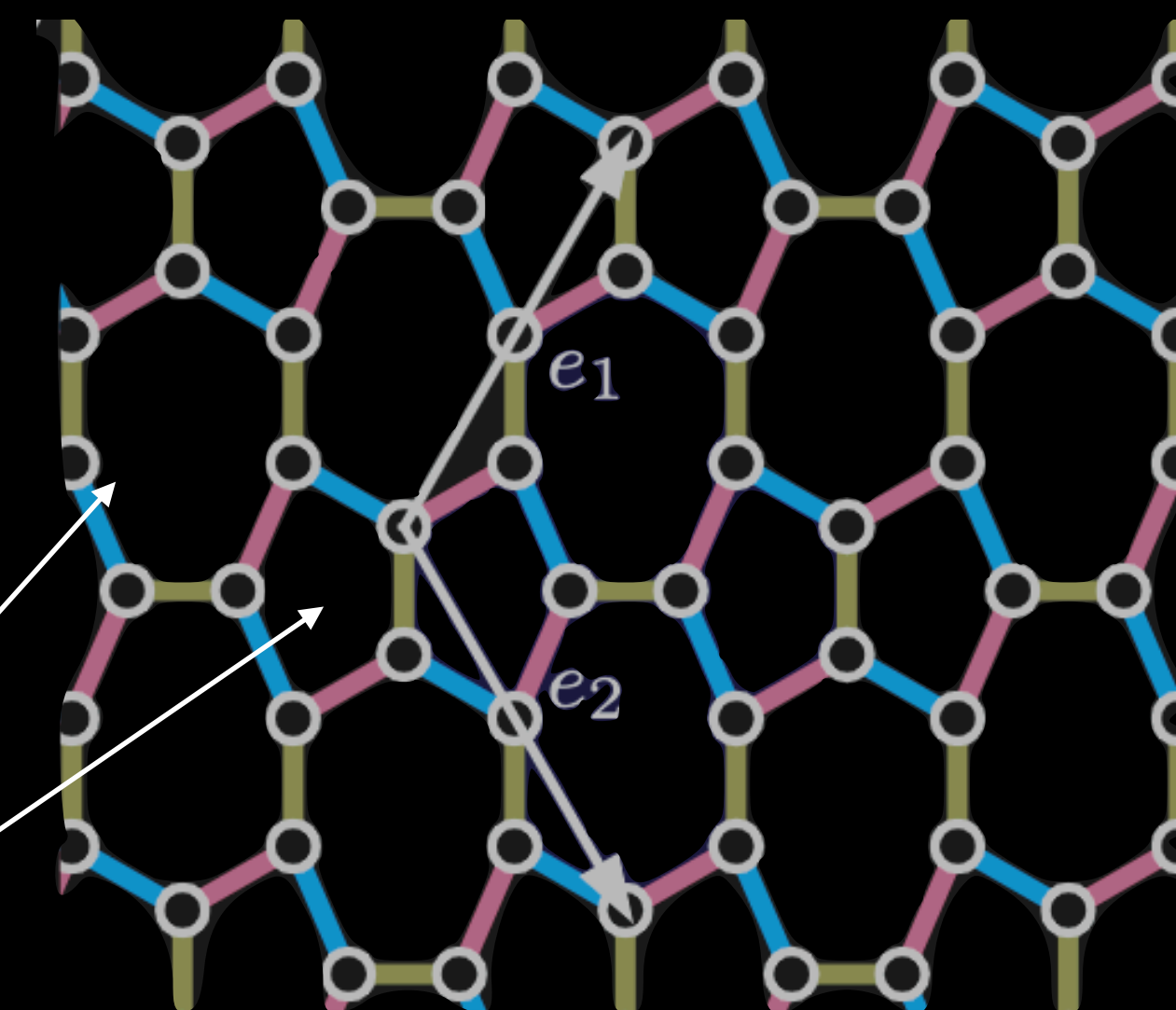
## Decorated Honeycomb

Yao and Kivelson PRL (2007)



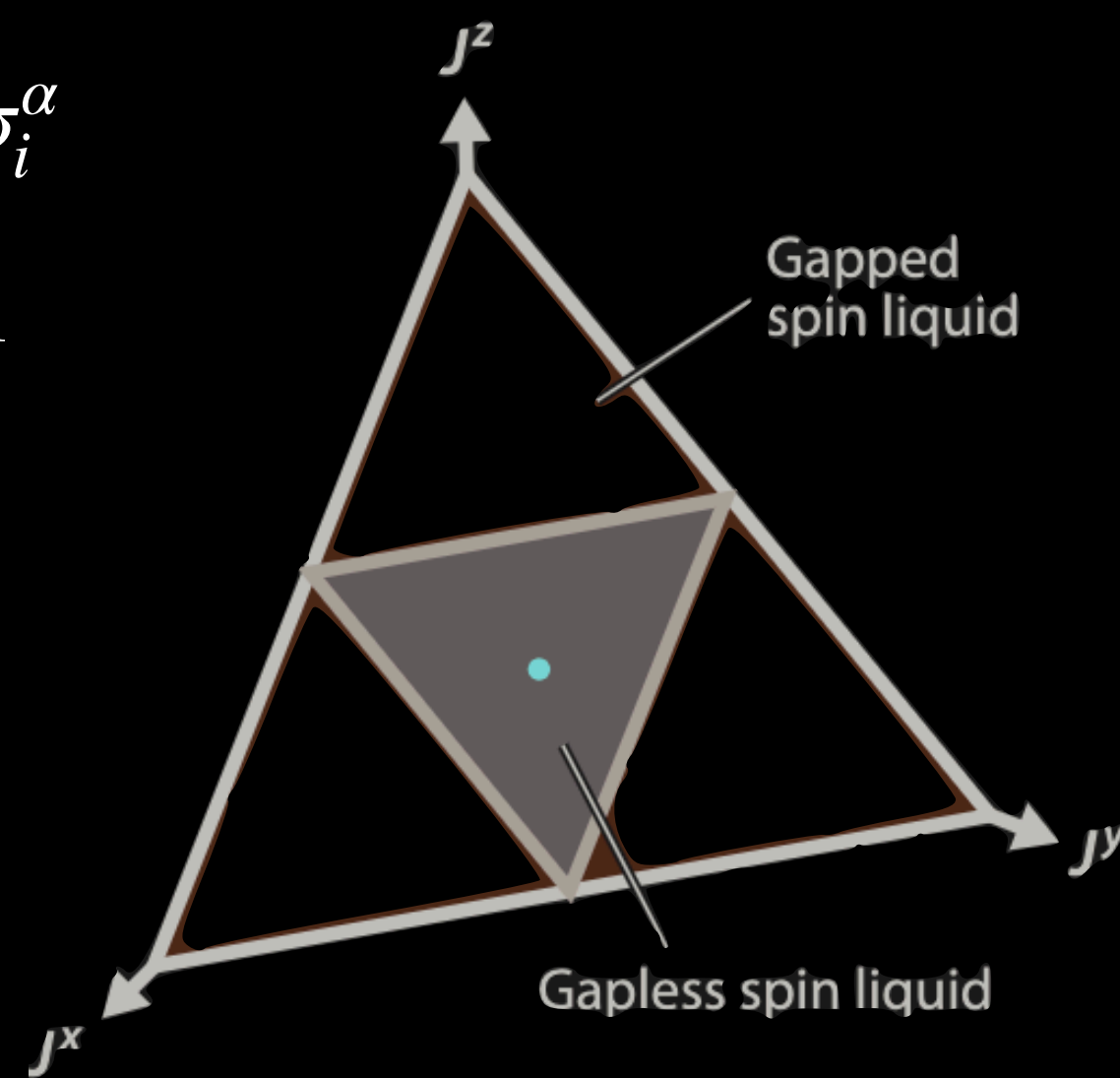
## Pentaheptite lattice

Peri et al PRB (2020)



$$W_p = \prod \sigma_i^\alpha$$

$$\phi_p = \pm 1$$



$$\phi_p = \pm 1$$

$$\phi_p = \pm i$$

Odd plaquettes break TRS



Gapped chiral spin-liquid!

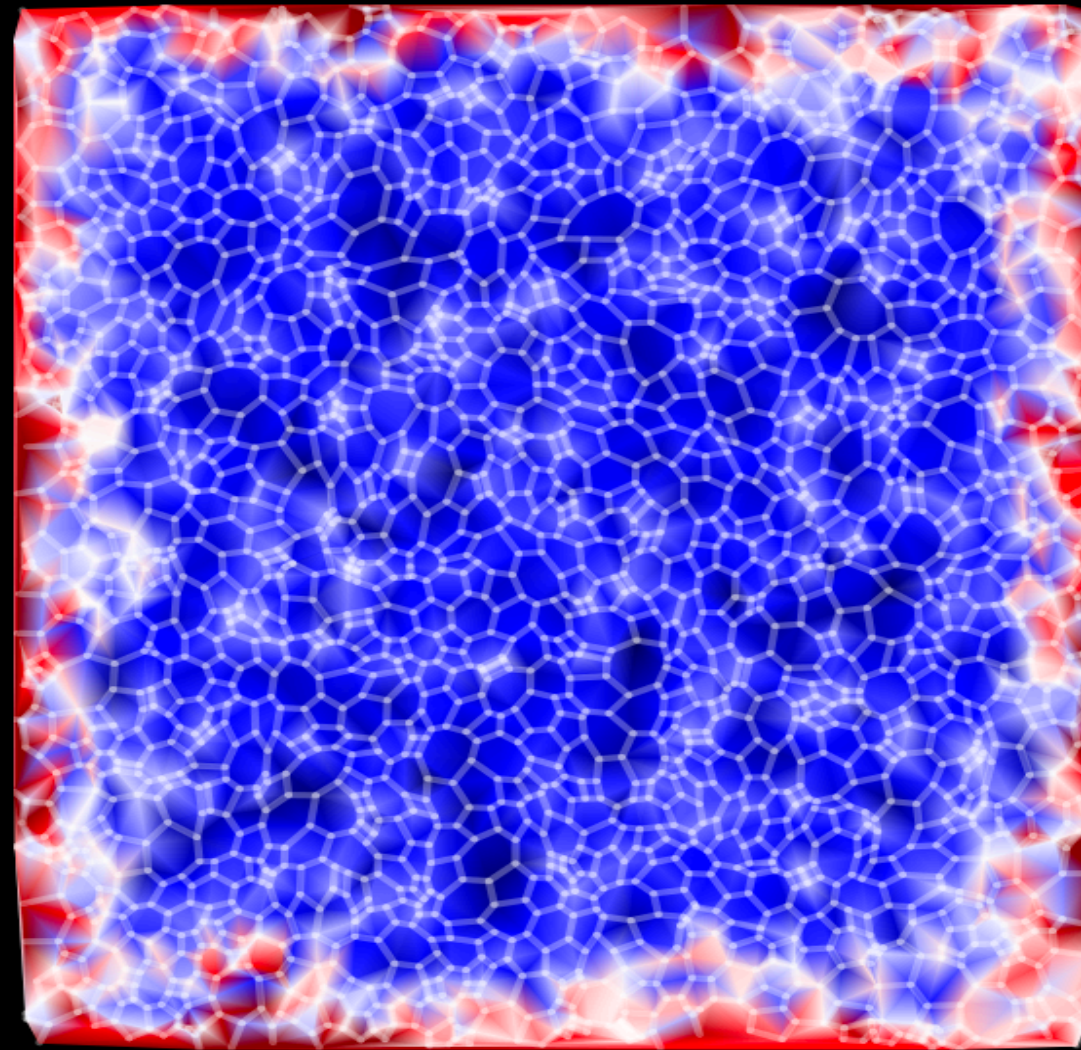
# Amorphous chiral spin liquid?

Gapped chiral spin-liquid!

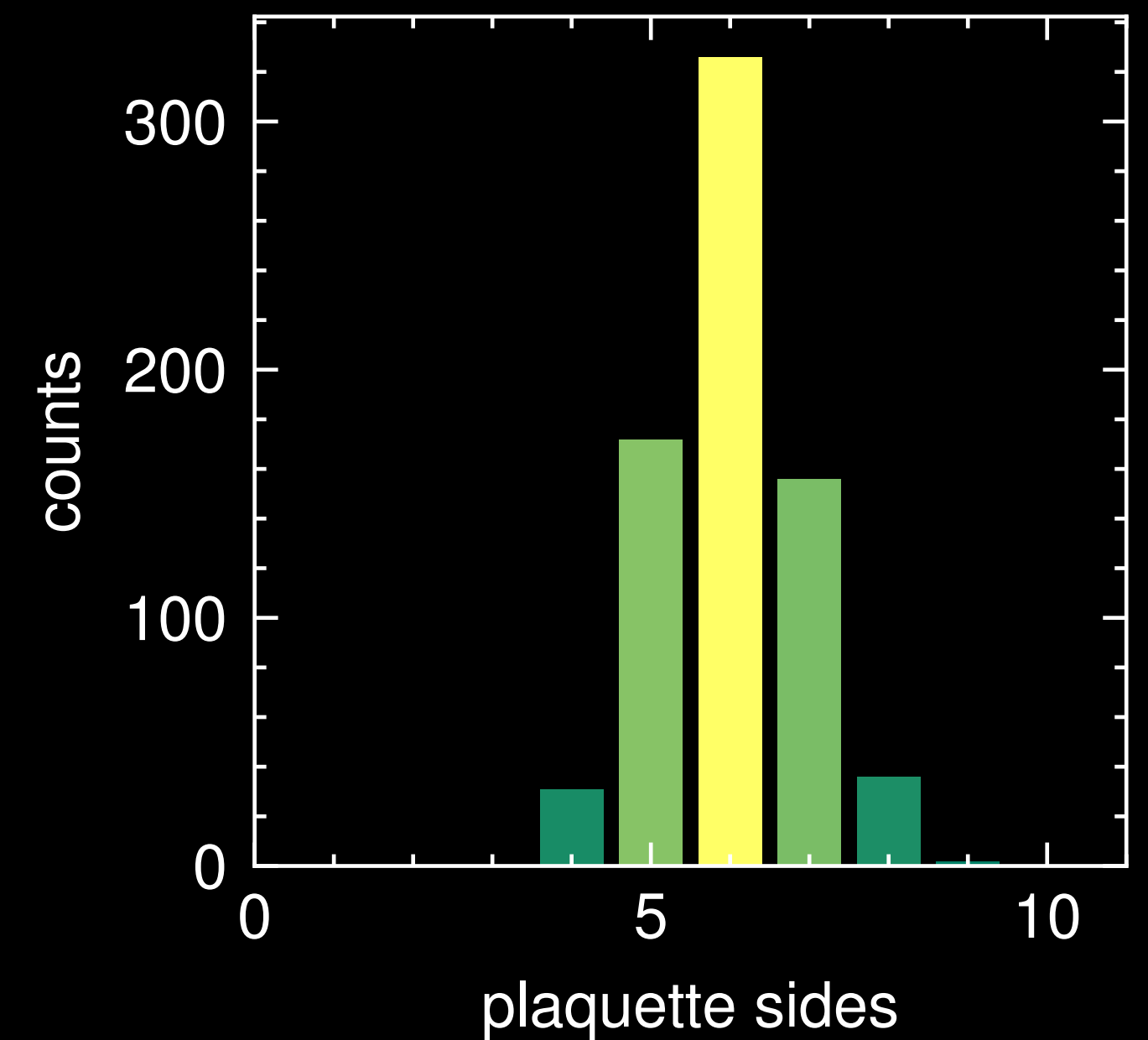
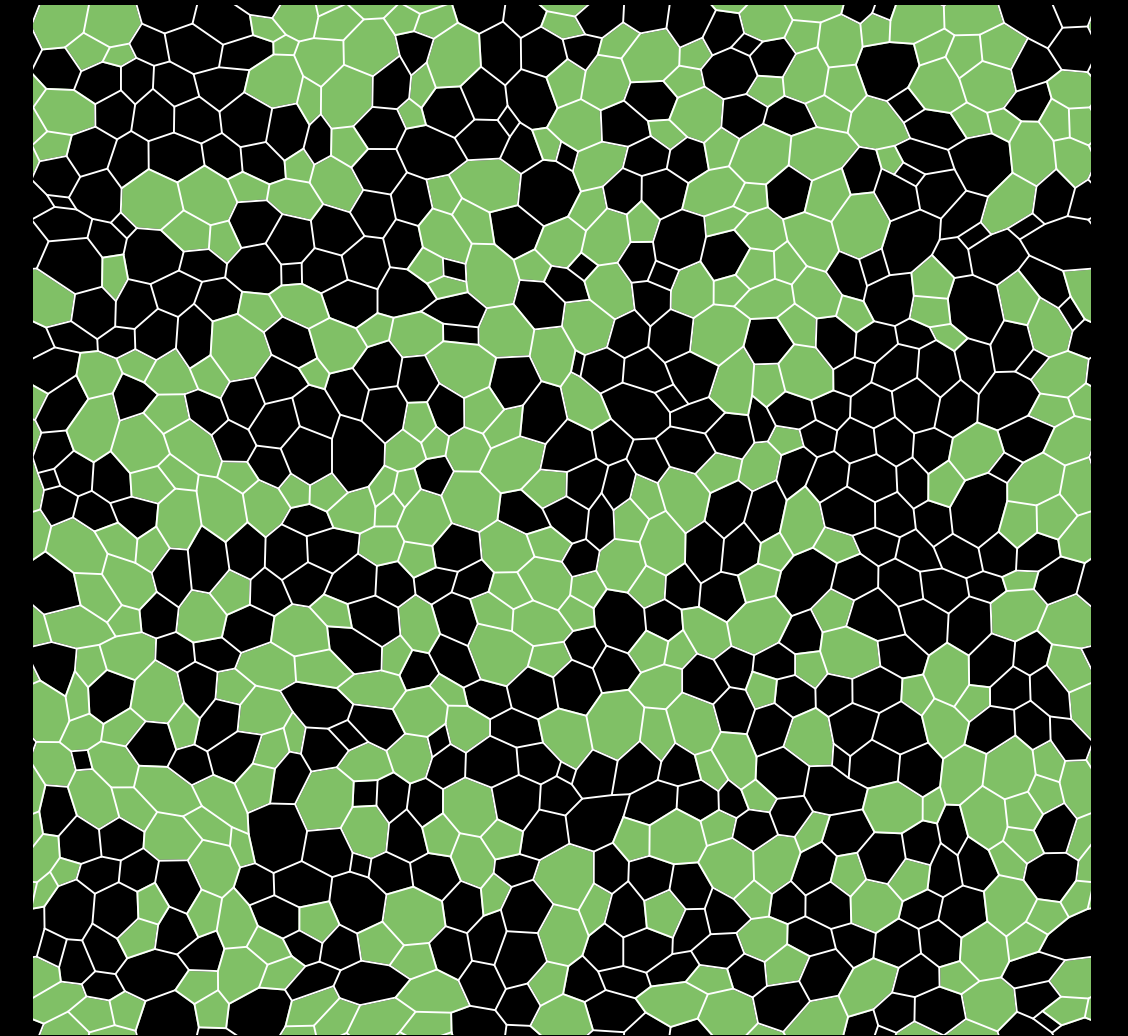
$$\phi_p = - (\pm i)^{n_{sides}}$$

G. Casella et al 2208.08246

Local Chern marker



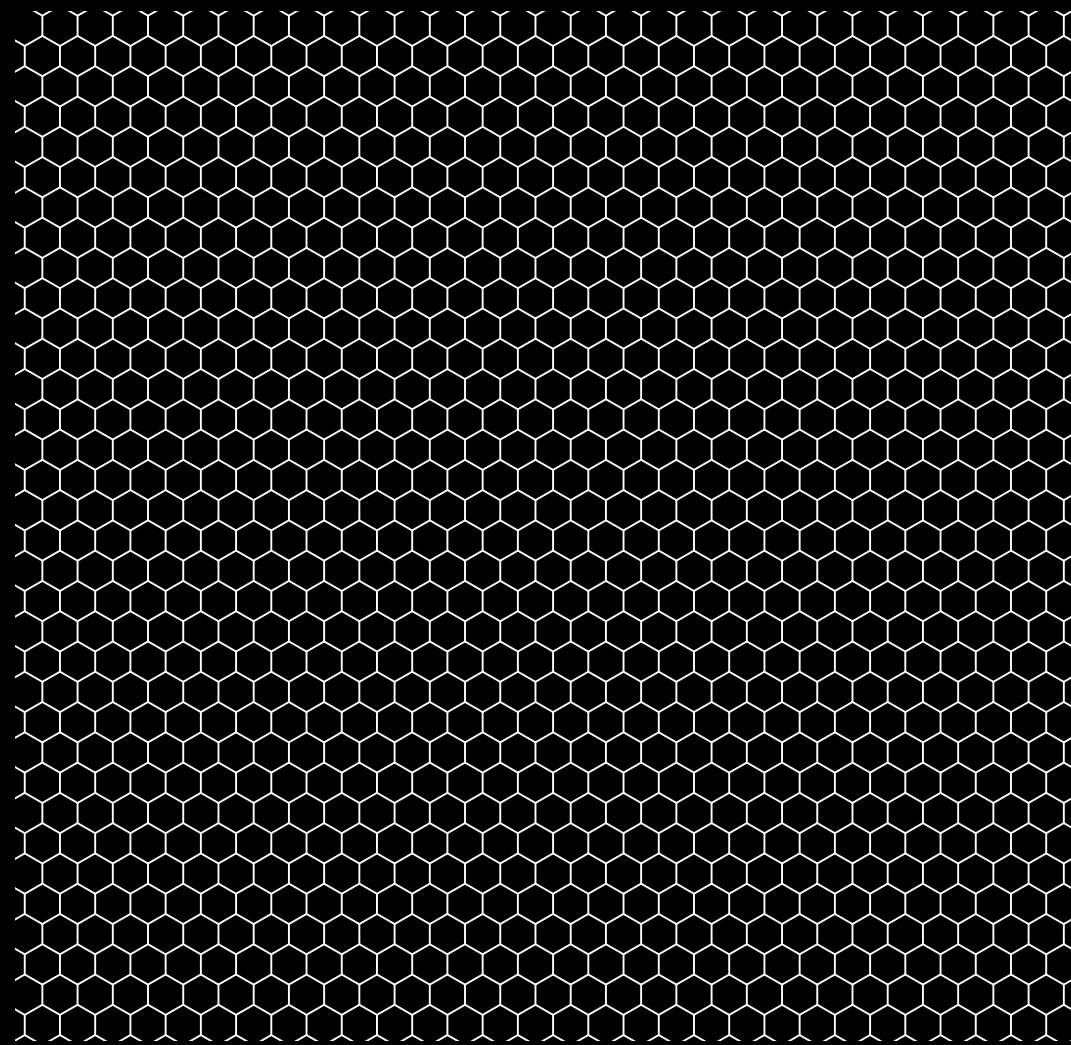
amorphous



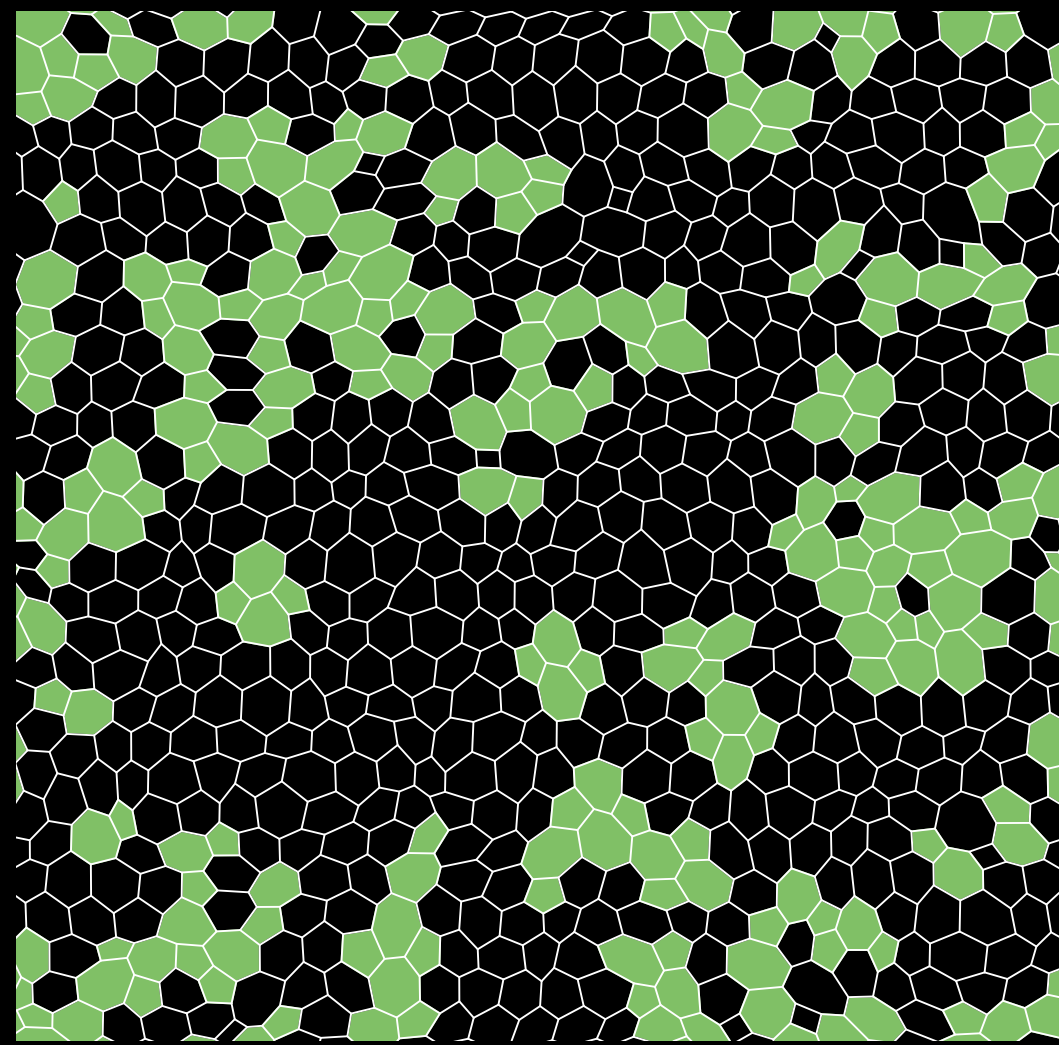
# Effect of the new knob?

AGG, C. Repellin 2210.13548

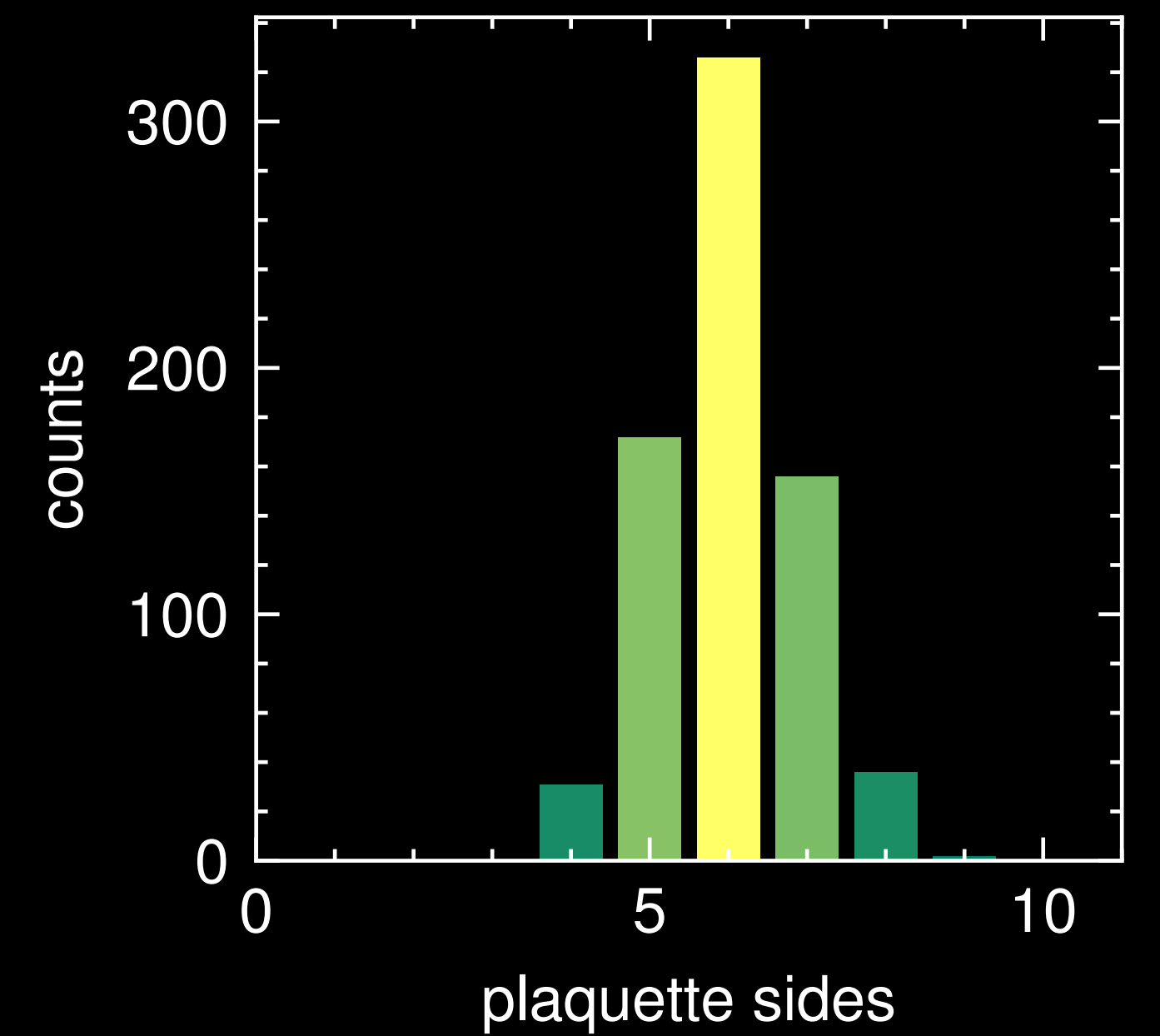
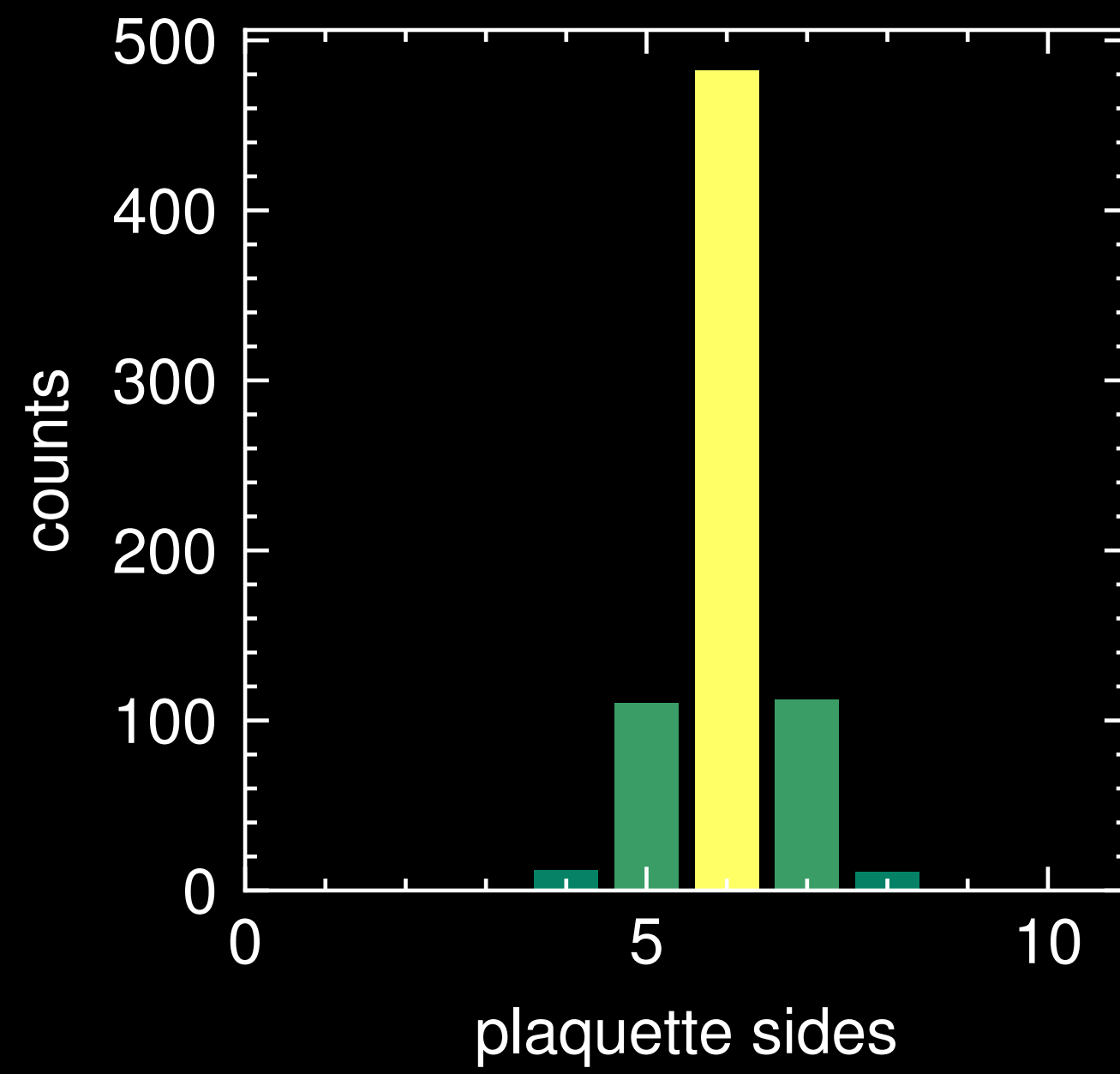
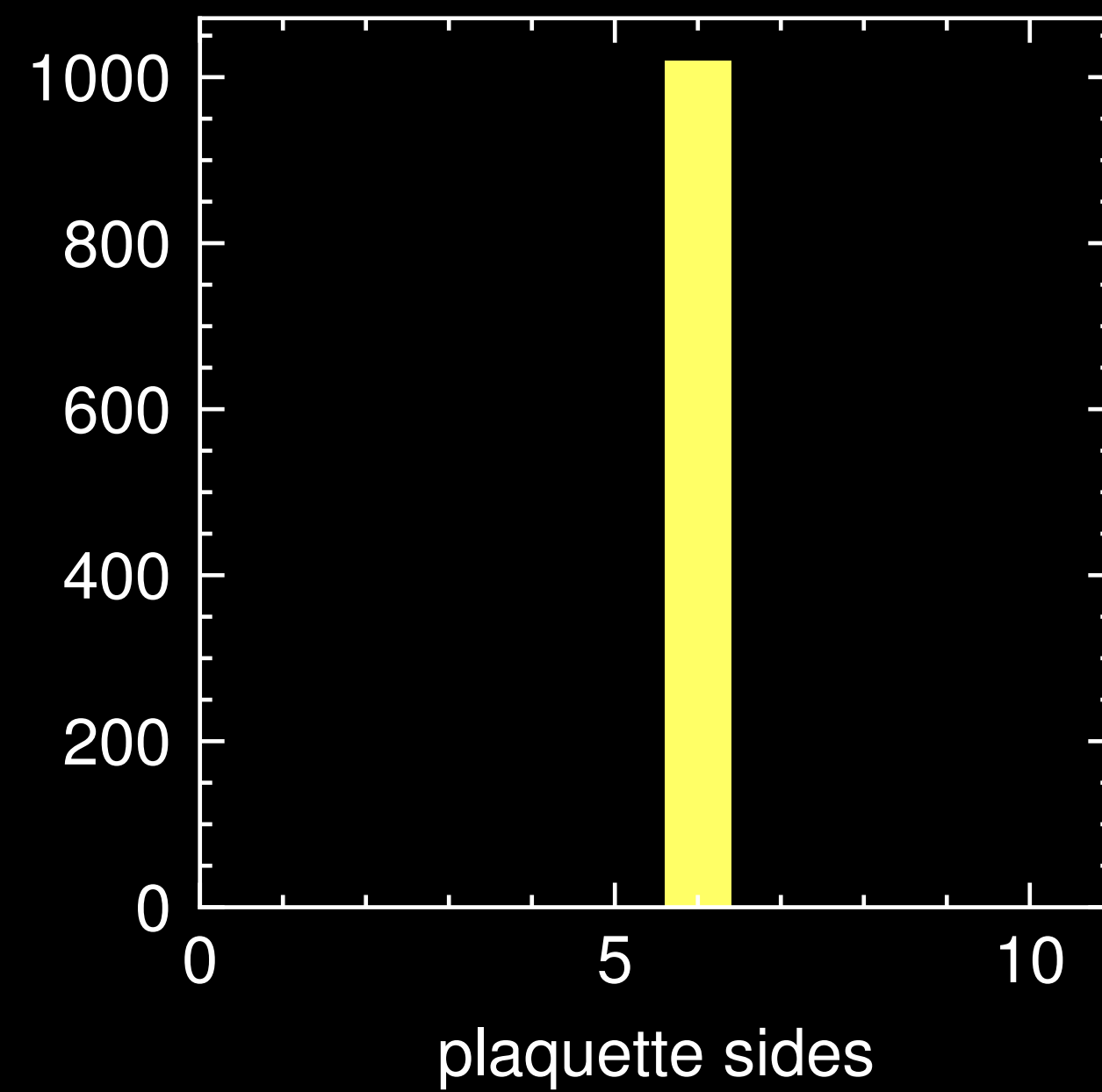
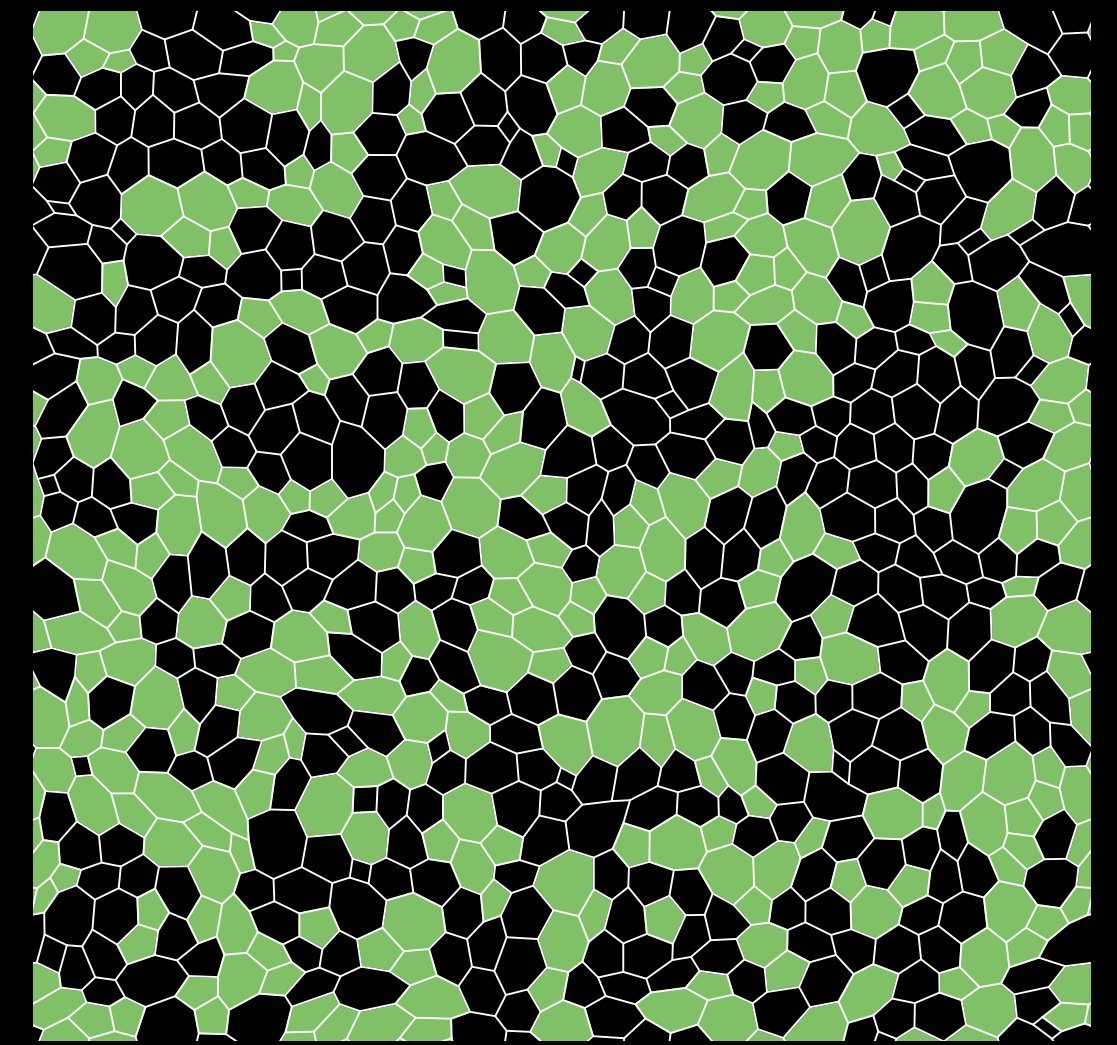
crystal



polycrystal



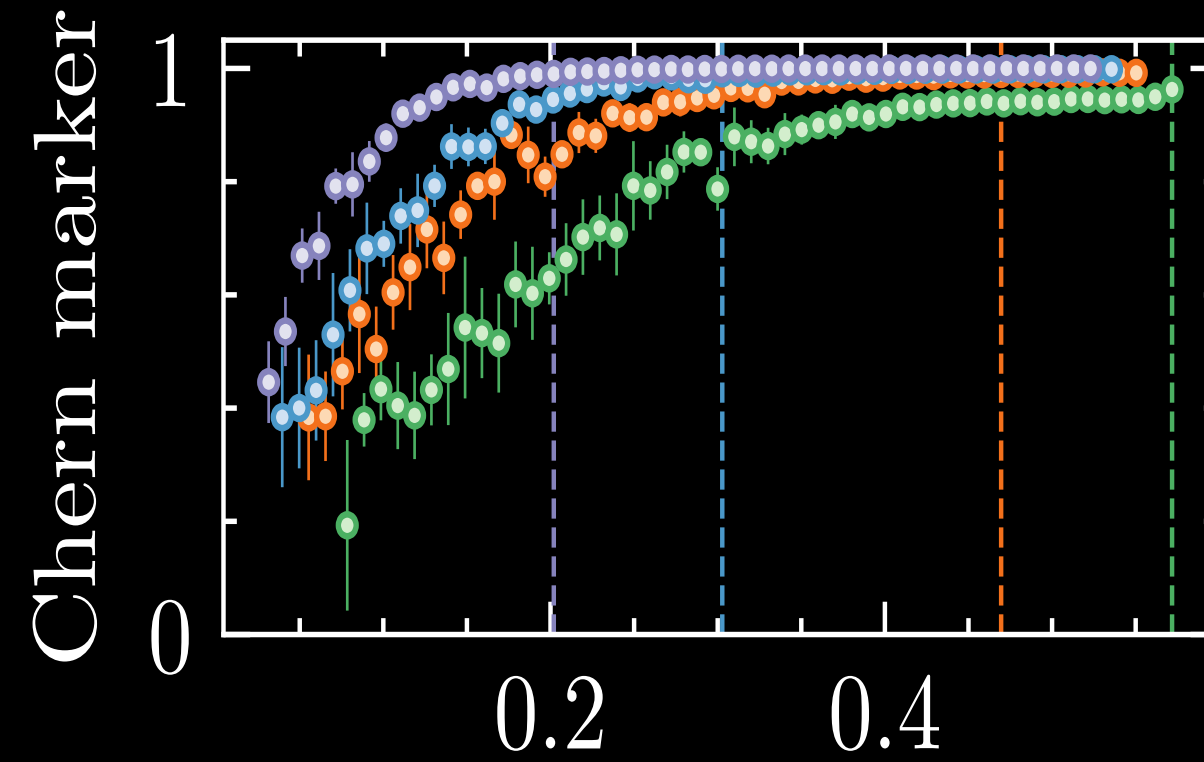
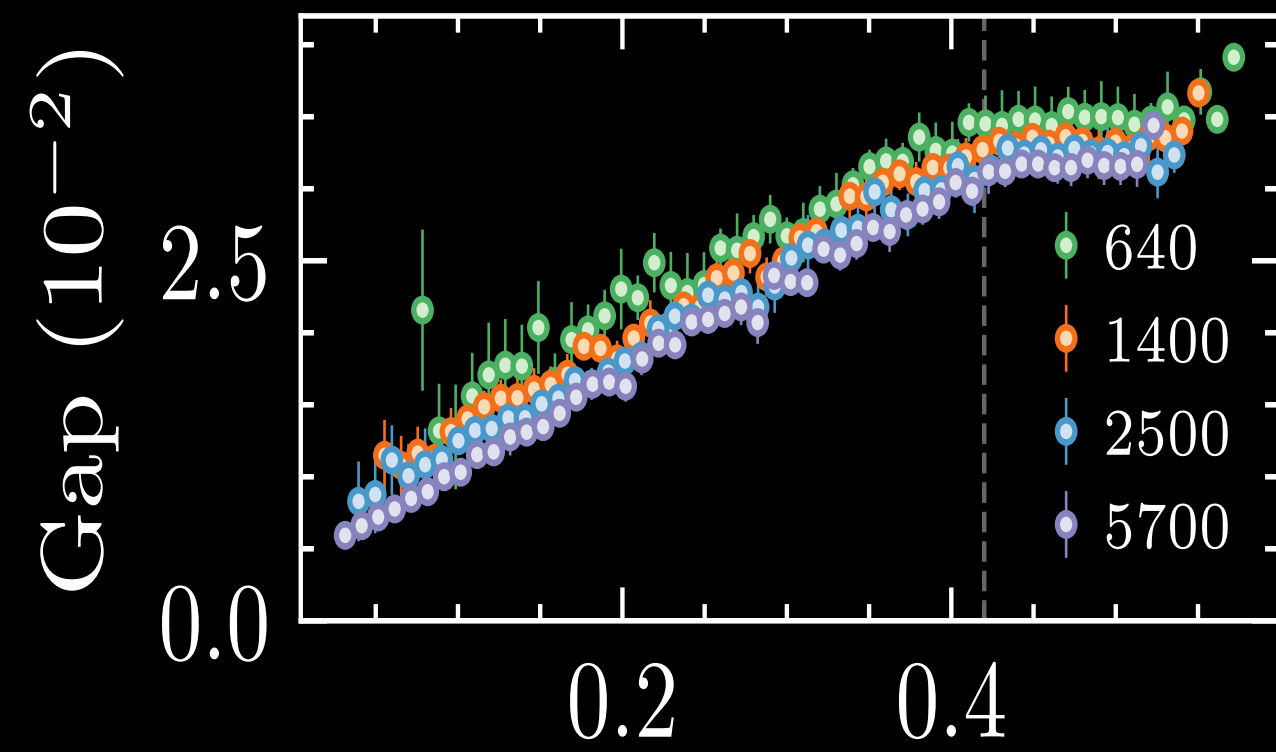
amorphous



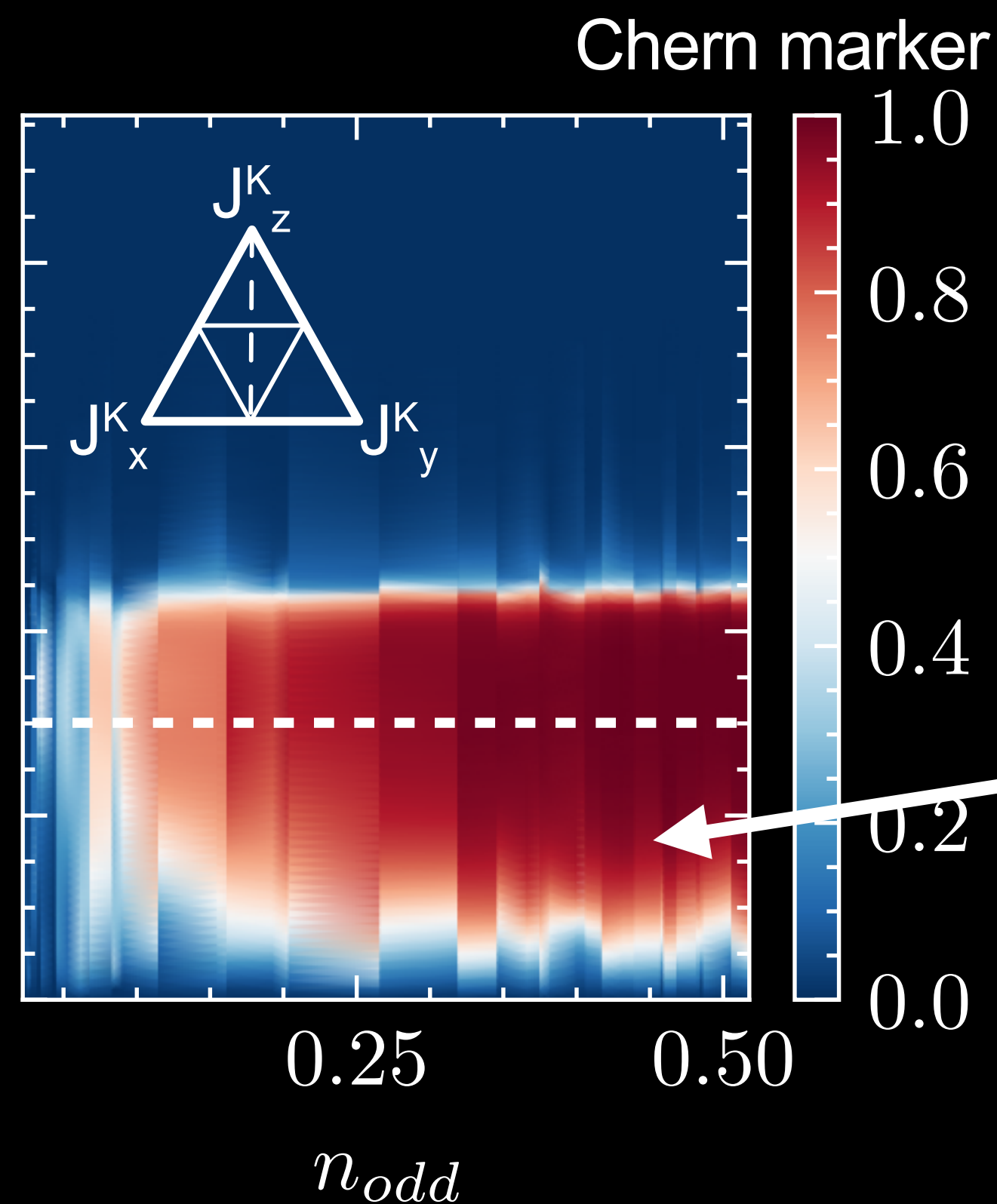
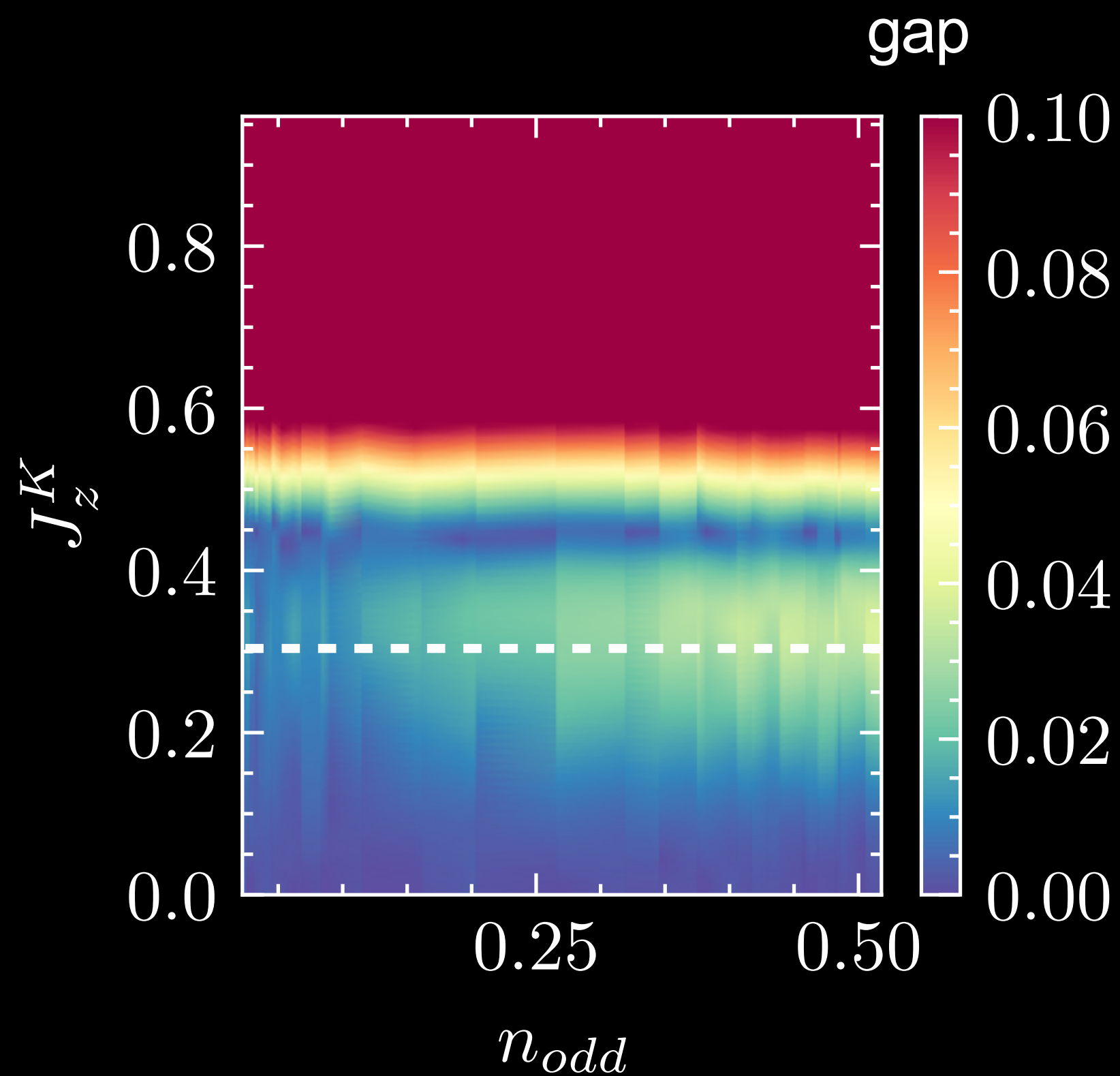


# A topological gap as disorder is increased

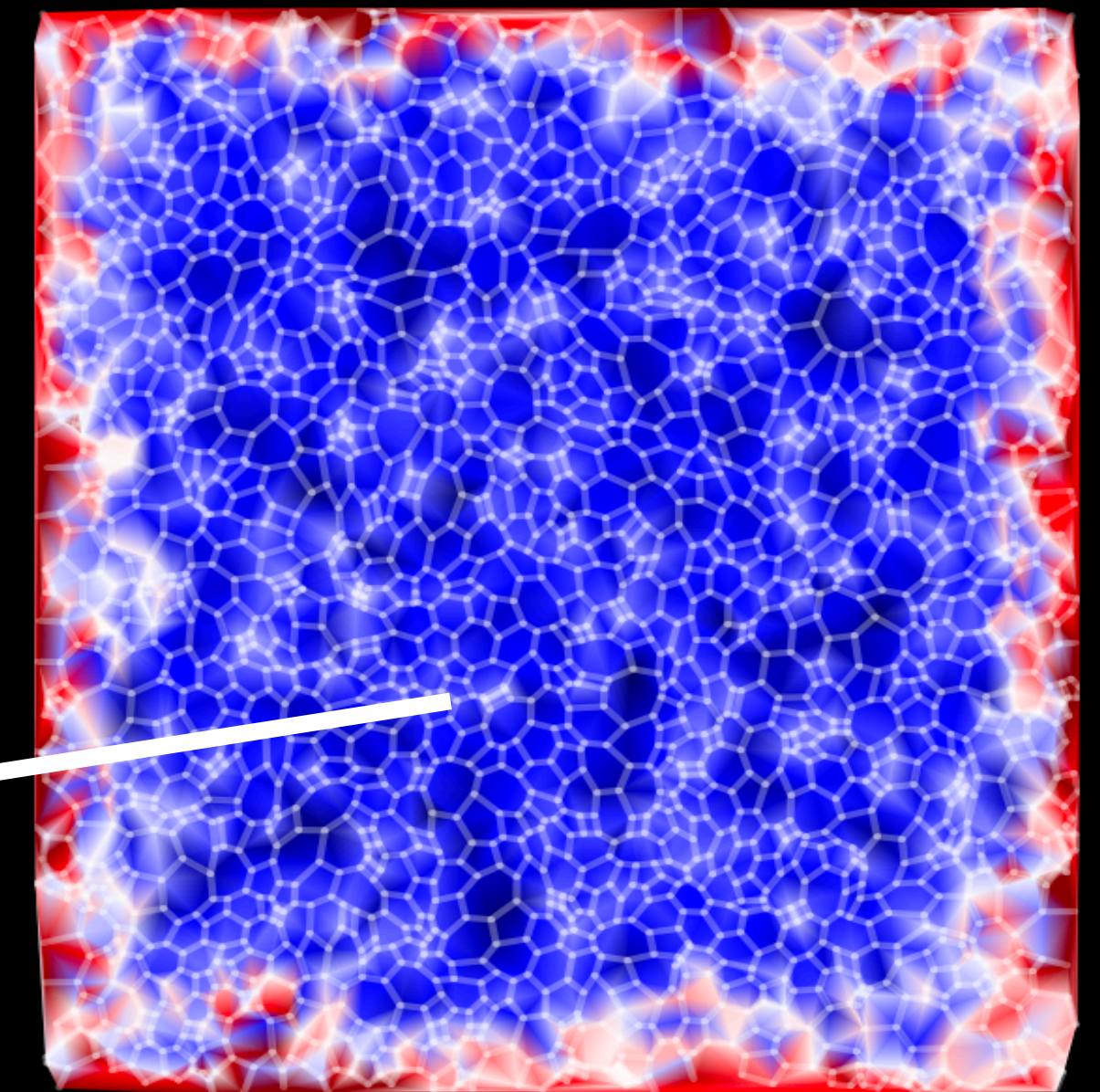
AGG, C. Repellin 2210.13548



small density of odd plaquettes is enough  
stable to Heisenberg interactions  
(confirmed by ED)



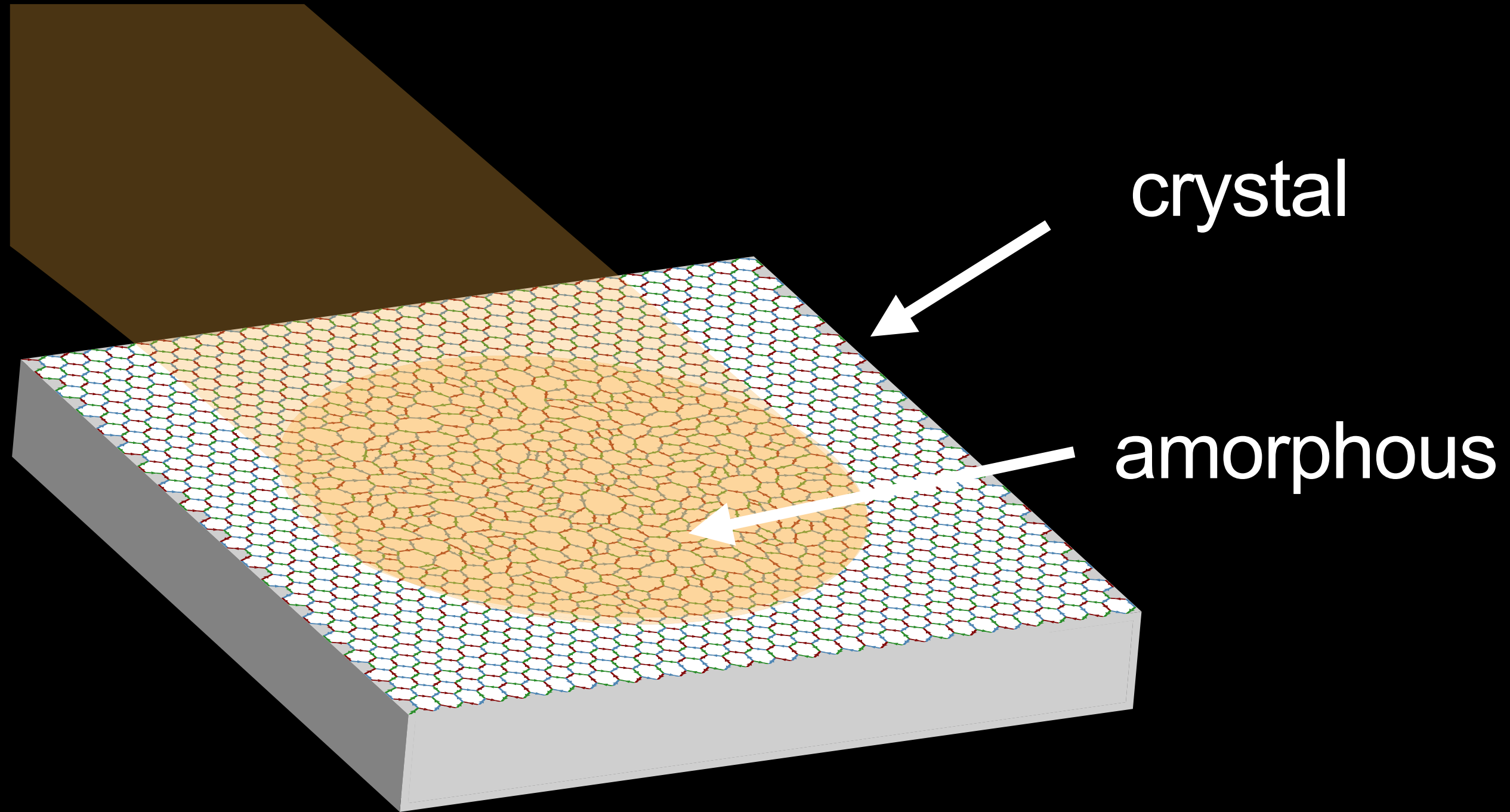
Local Chern marker



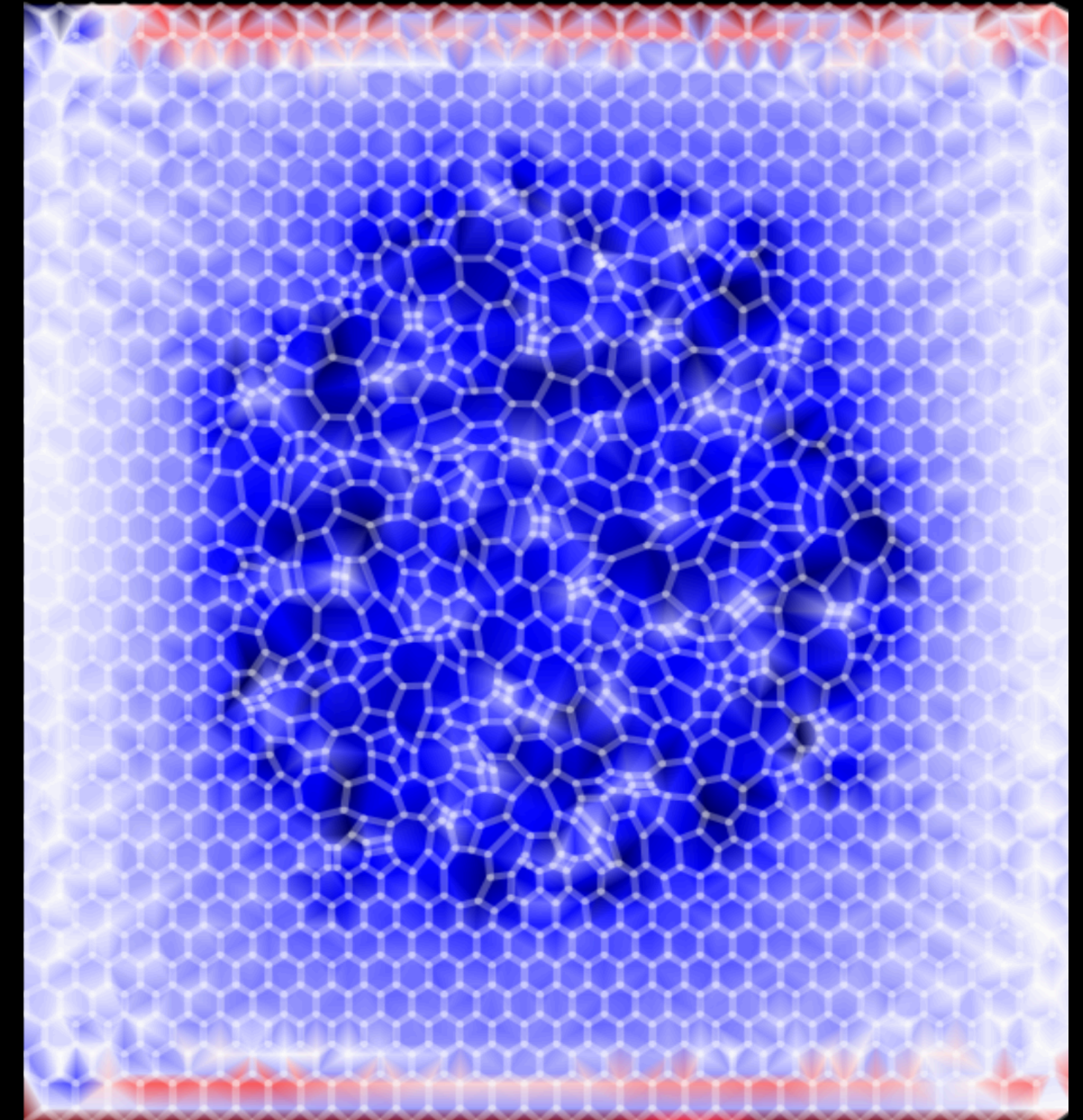
# A new knob to control

AGG, C. Repellin 2210.13548

**focused ion beam**



Local Chern marker

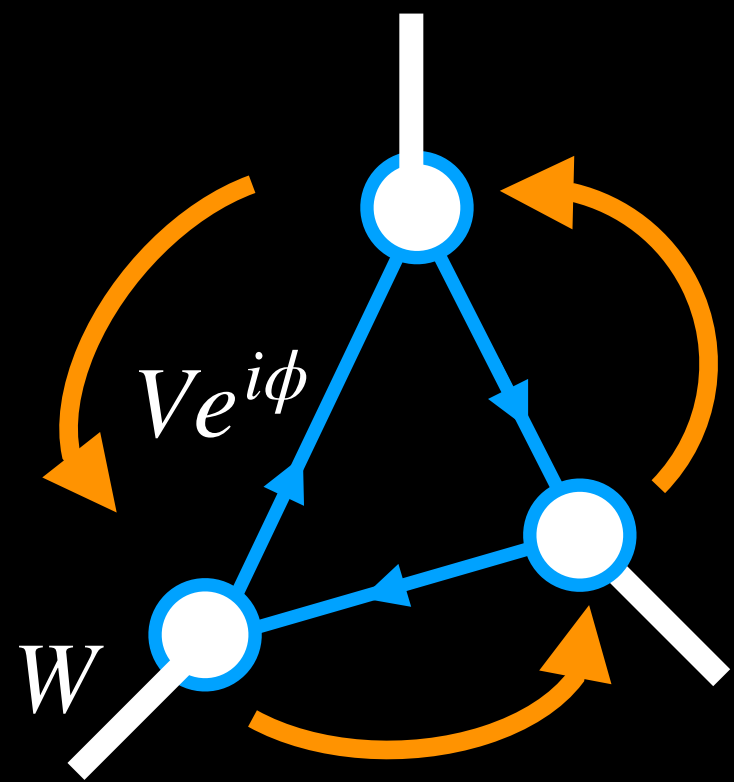


# Conclusions

## Finding amorphous solids efficiently

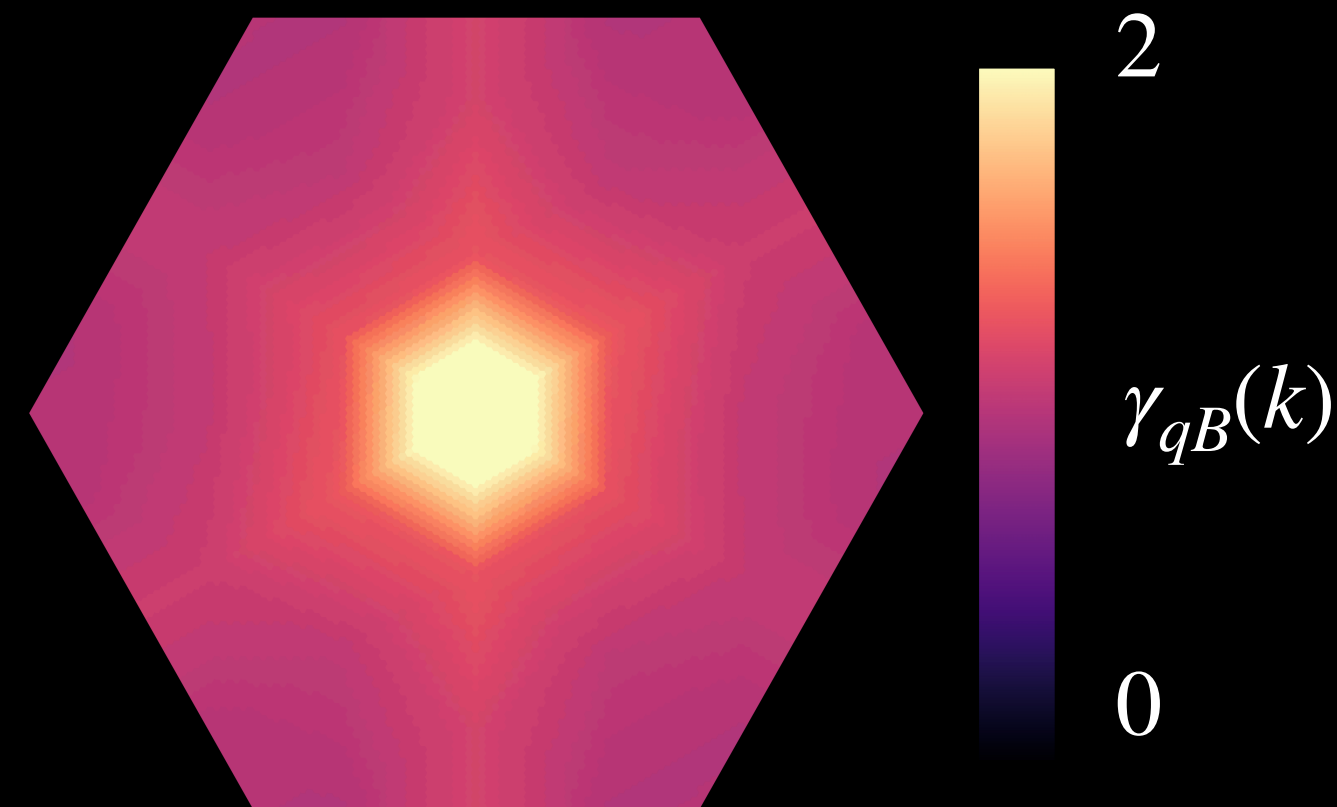
### Symmetry indicators

Q. Marsal, D. Varjas, AGG PNAS, (2020)



### Structural spillage

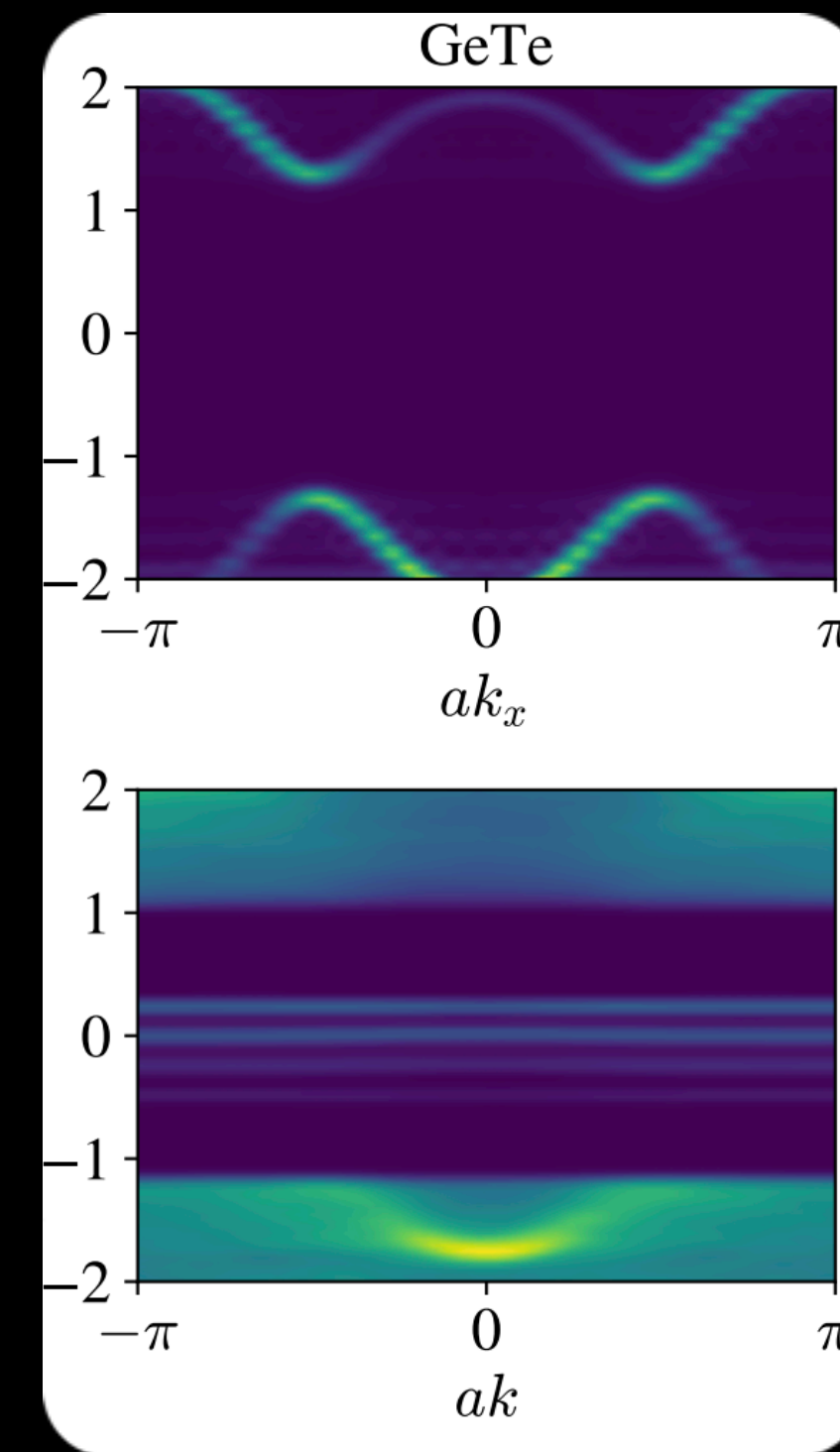
D. Muñoz-Segovia, et al arXiv: 2301.02686



## New control mechanisms

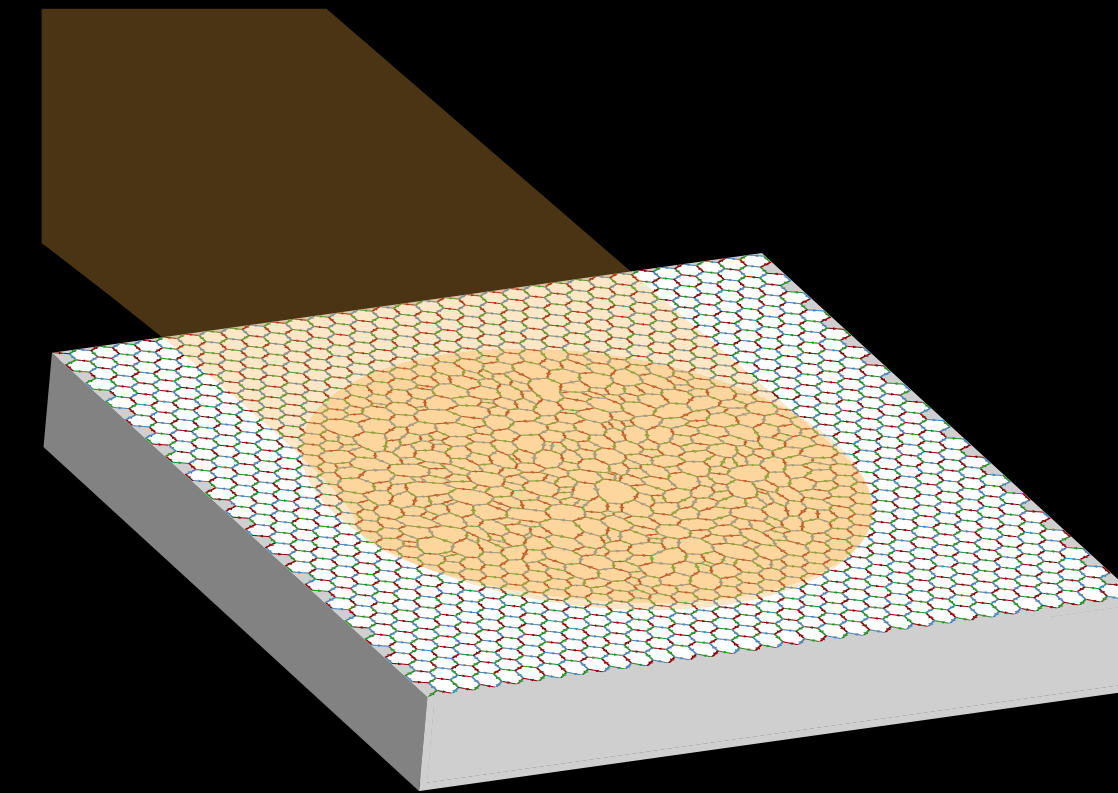
### Controllable flat-bands

Q. Marsal, D. Varjas, Phys. Rev. B (2023)



### Chiral spin liquids

AGG, C. Repellin 2210.13548



Exp: Corbae et al, AGG, Lanzara, Hellmann Nat Materials (2023)  
Cyocis, Marsal et al, Hellmann, AGG, Lanzara 2302.05945

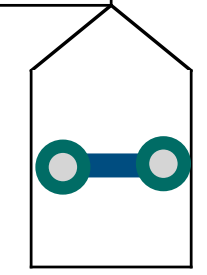
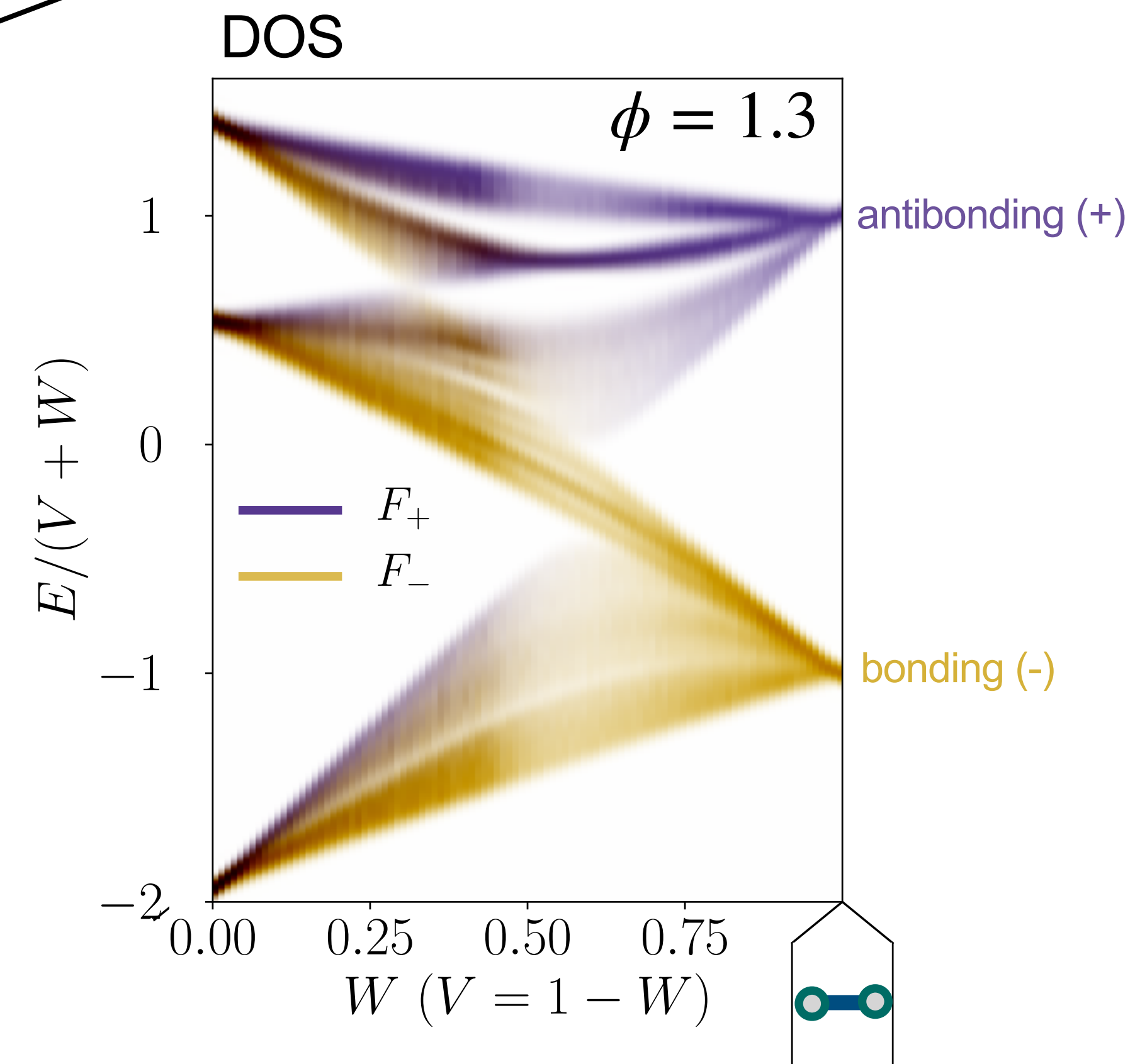
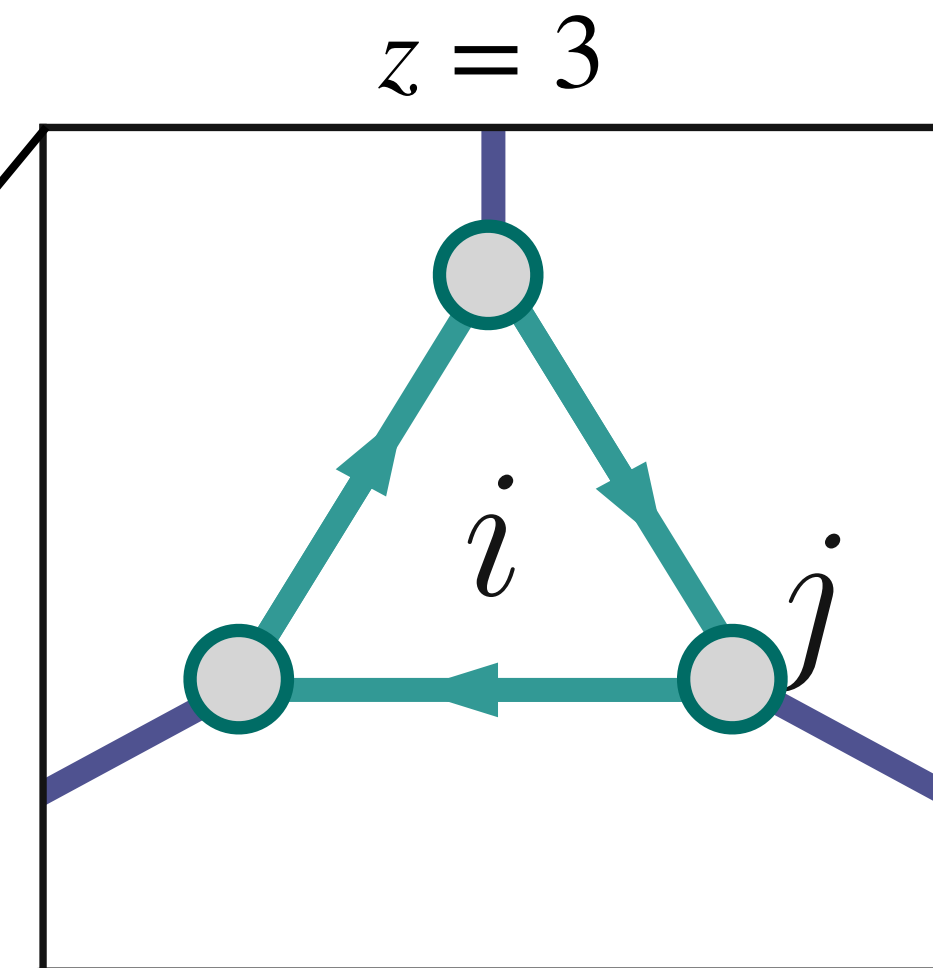
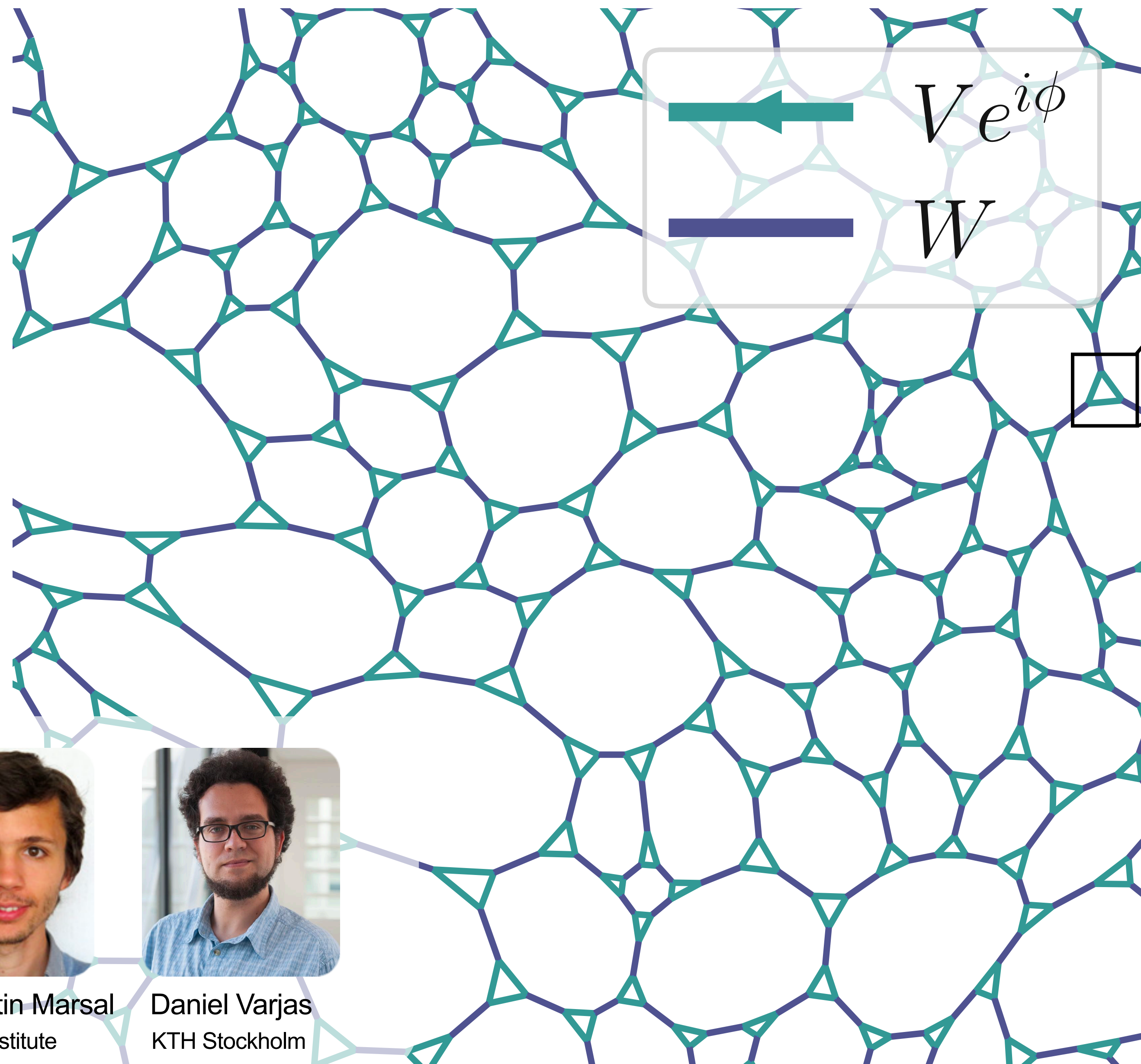
Review: P. Corbae, J. Hannukainen, Q. Marsal, D. Muñoz-Segovia, AGG  
arXiv:2301.04176 (EPL in press)



Technical details: Symmetry indicators

# Topological Weaire-Thorpe model

Q. Marsal, D. Varjas, AGG PNAS, (2020)



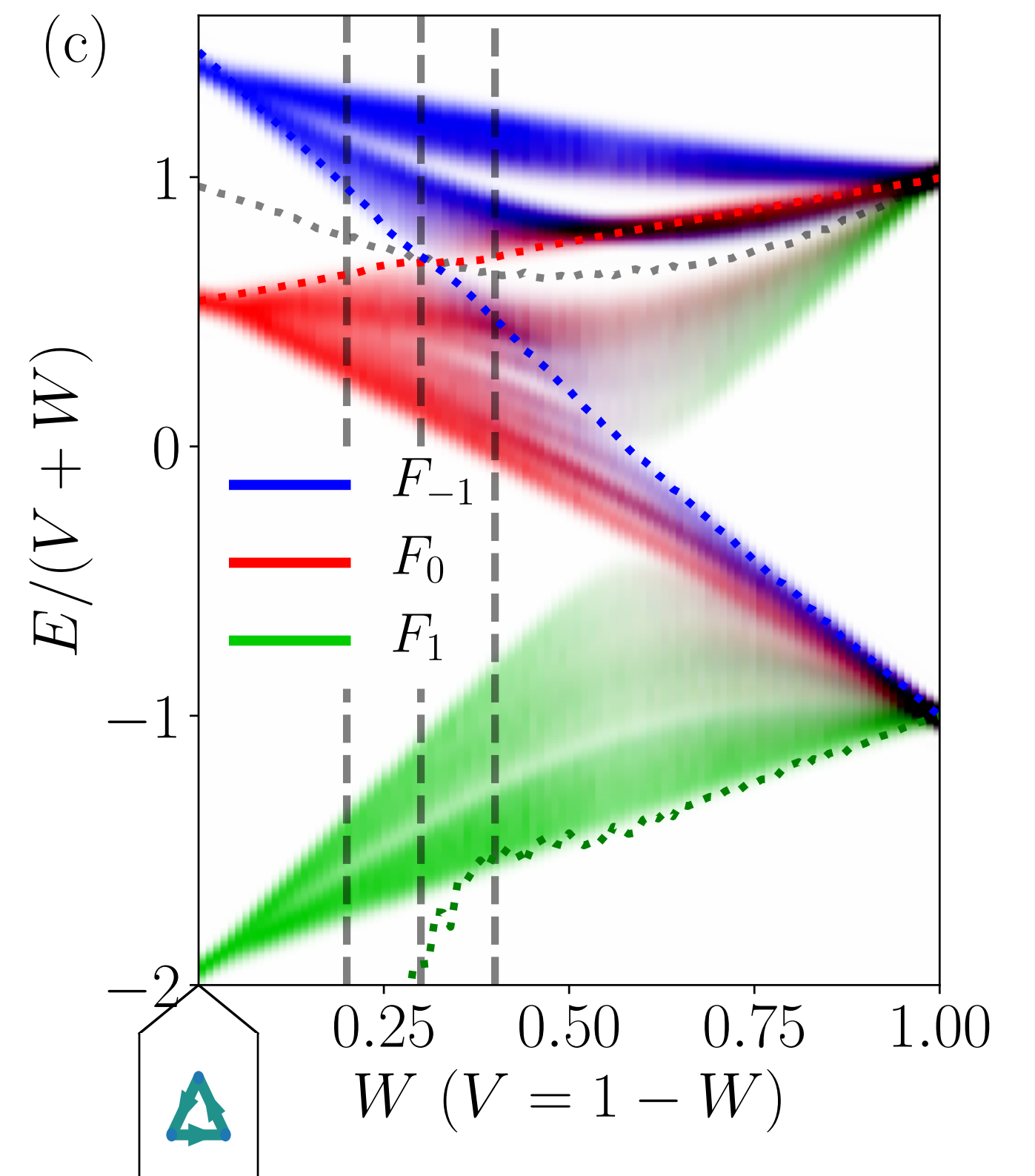
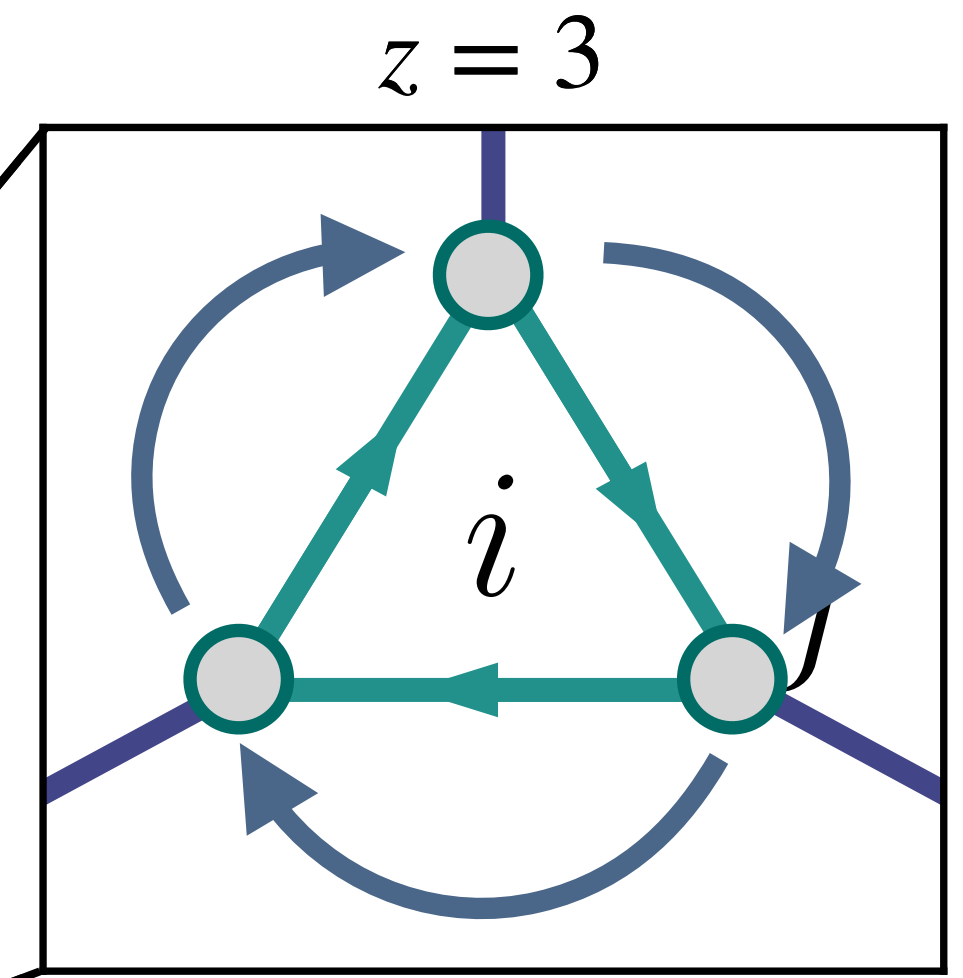
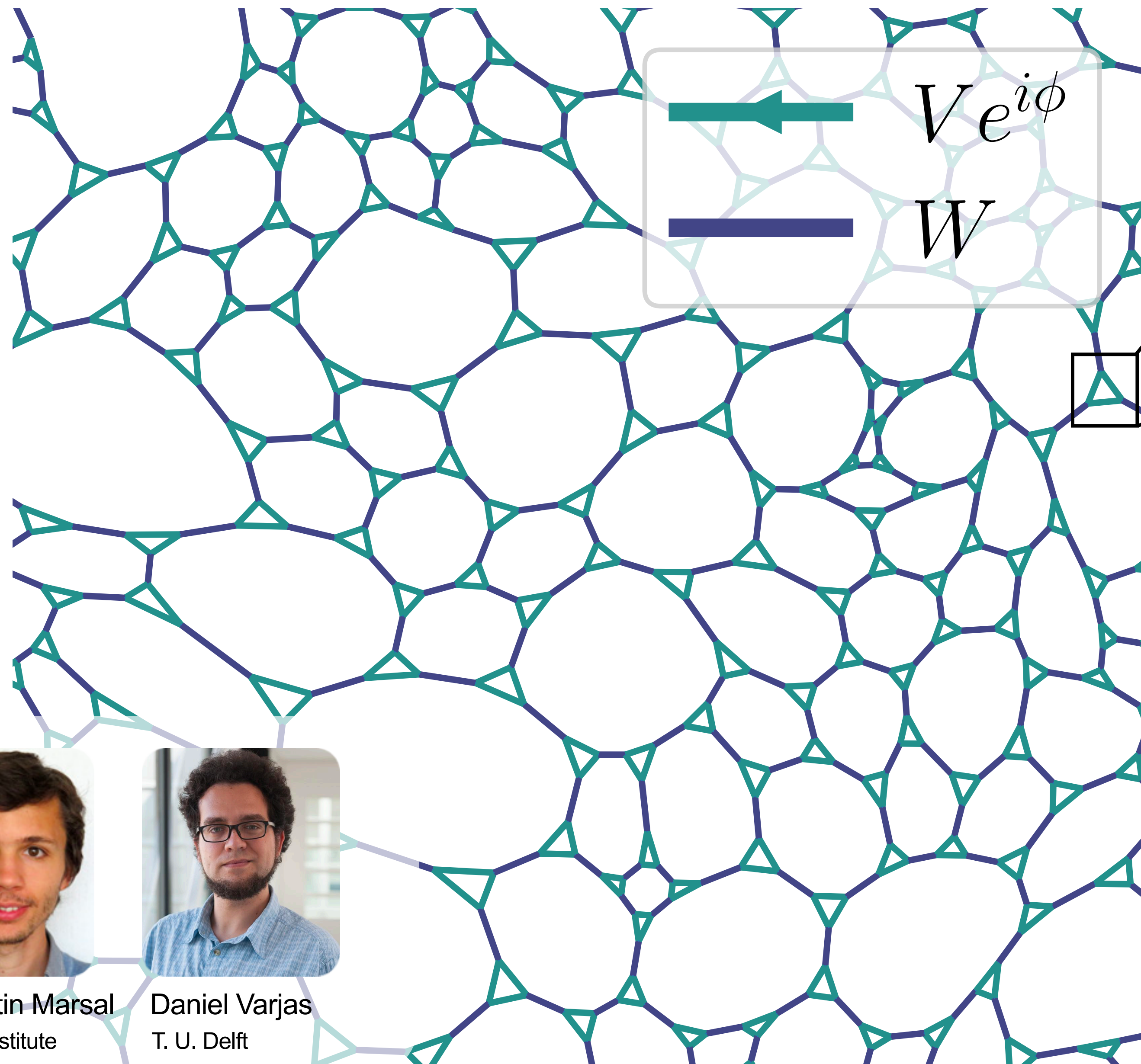
Quentin Marsal  
Néel Institute



Daniel Varjas  
KTH Stockholm

# Topological Weaire-Thorpe model

Q. Marsal, D. Varjas, AGG PNAS, (2020)



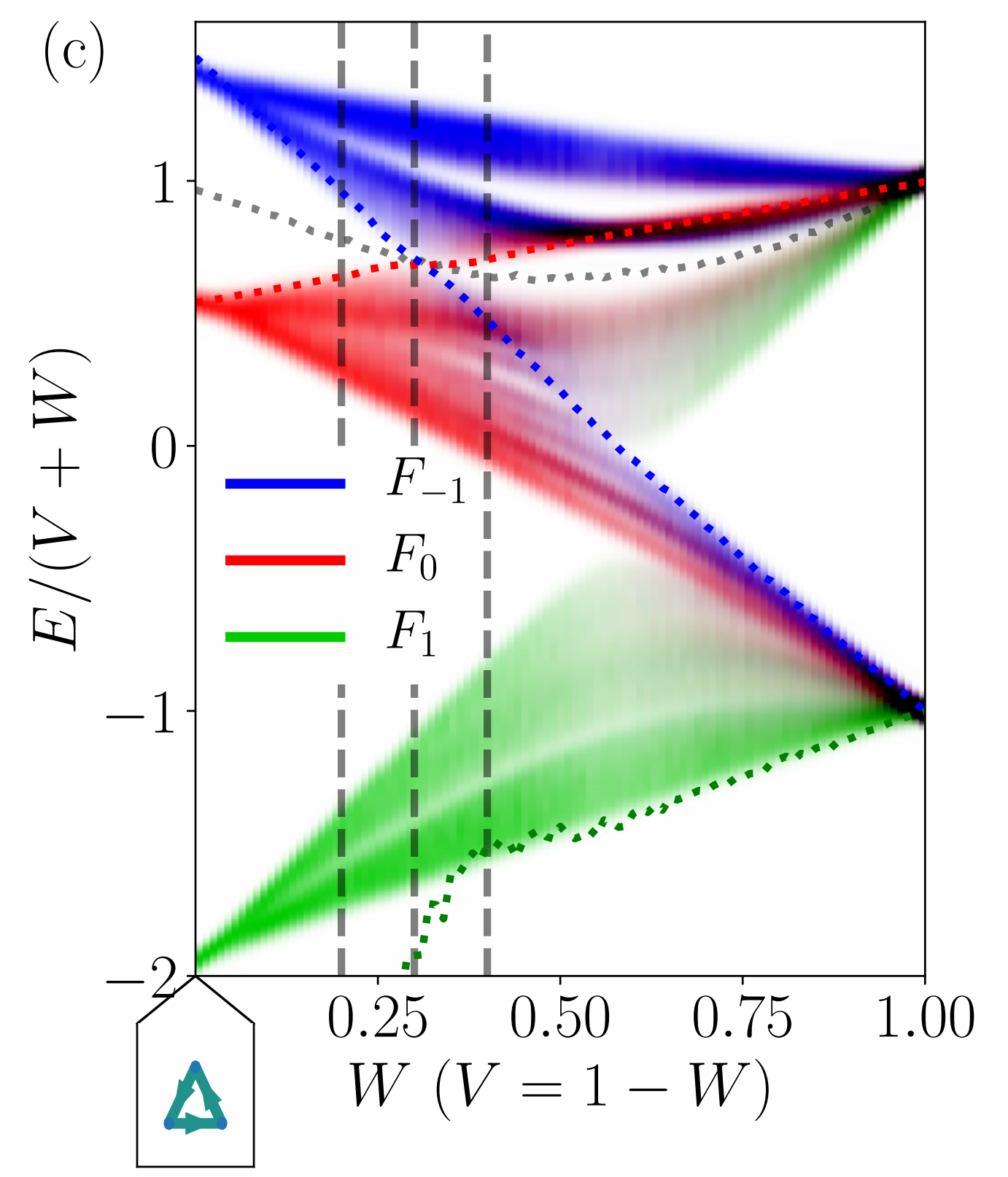
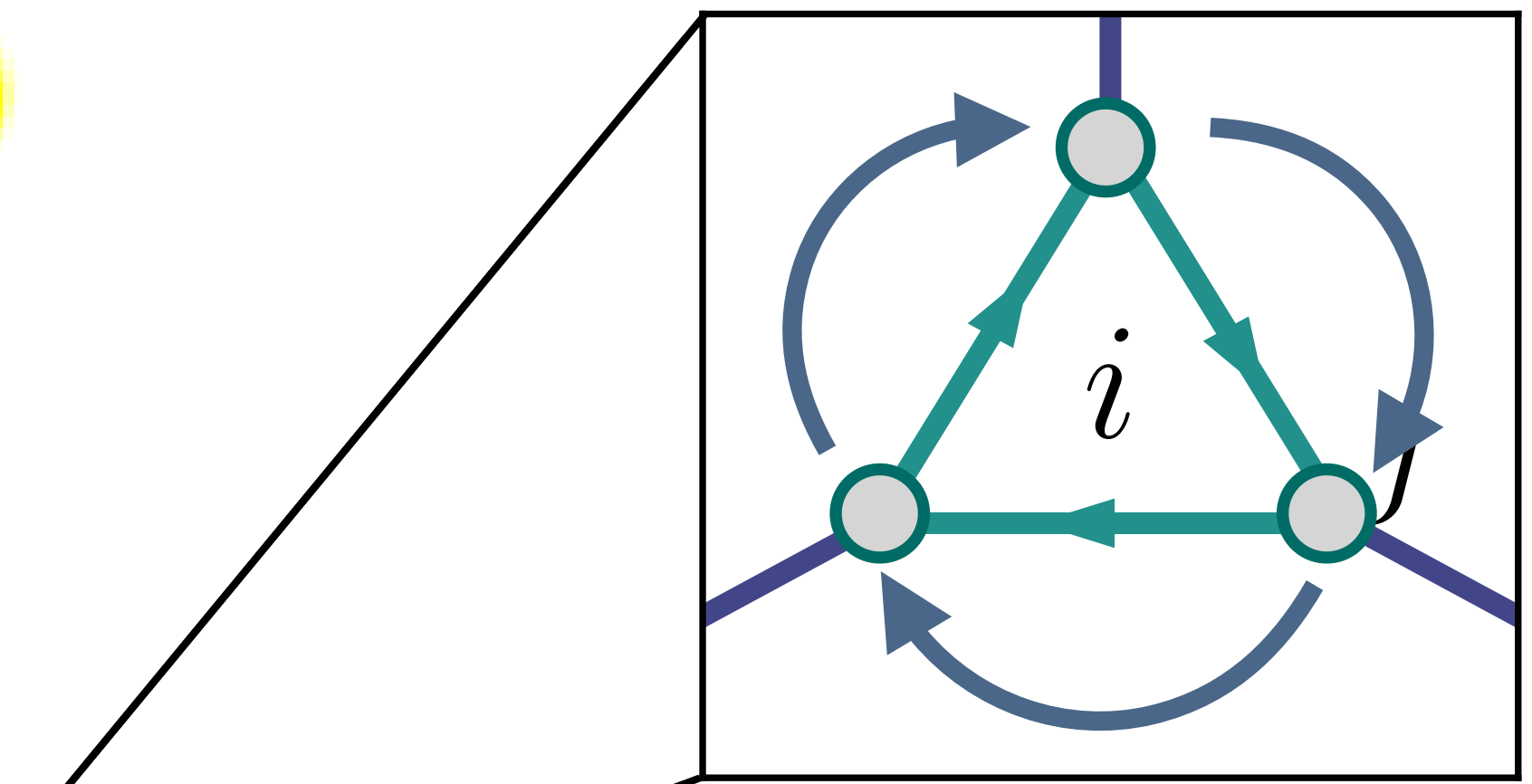
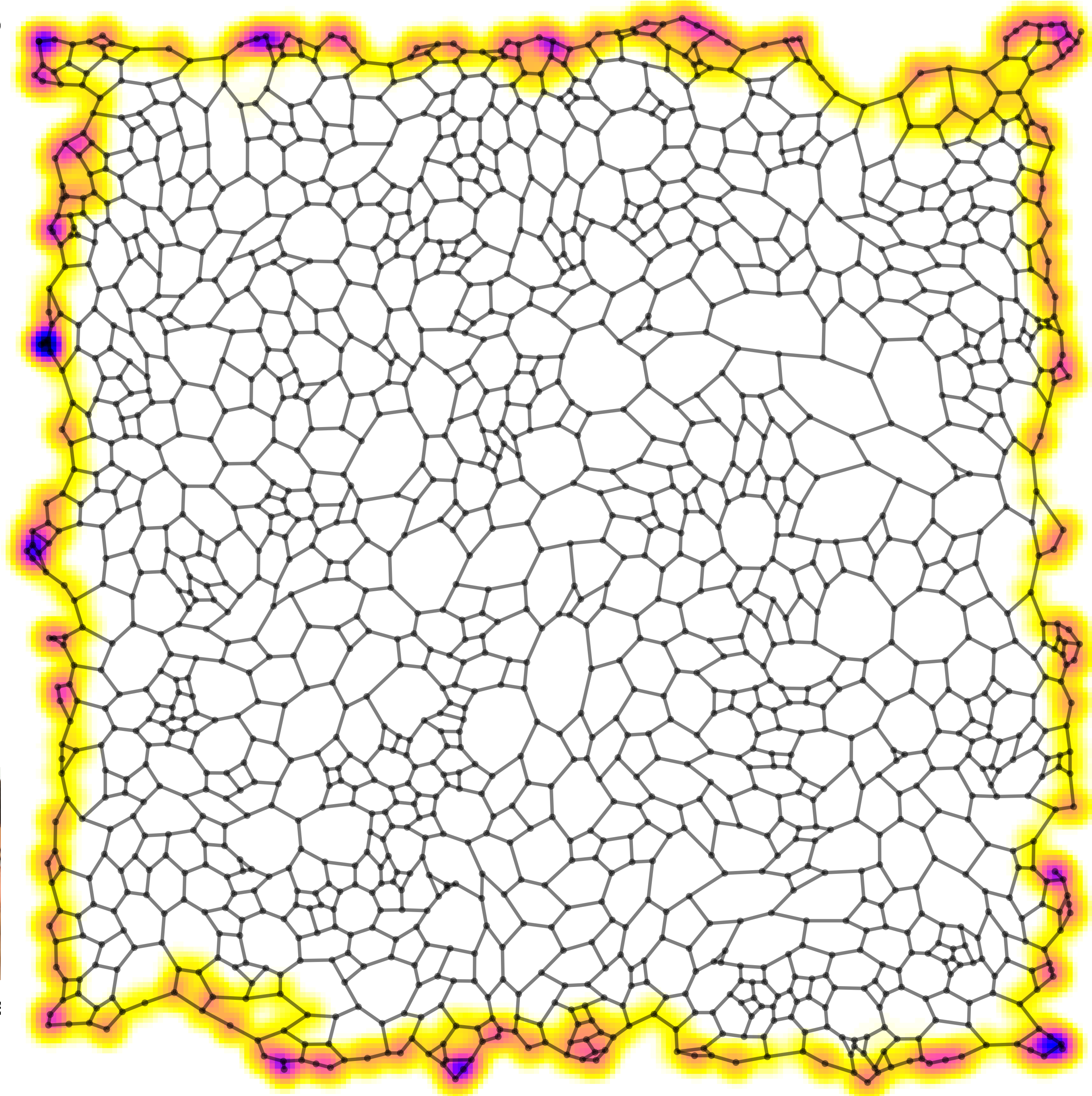
Quentin Marsal  
Néel Institute



Daniel Varjas  
T. U. Delft

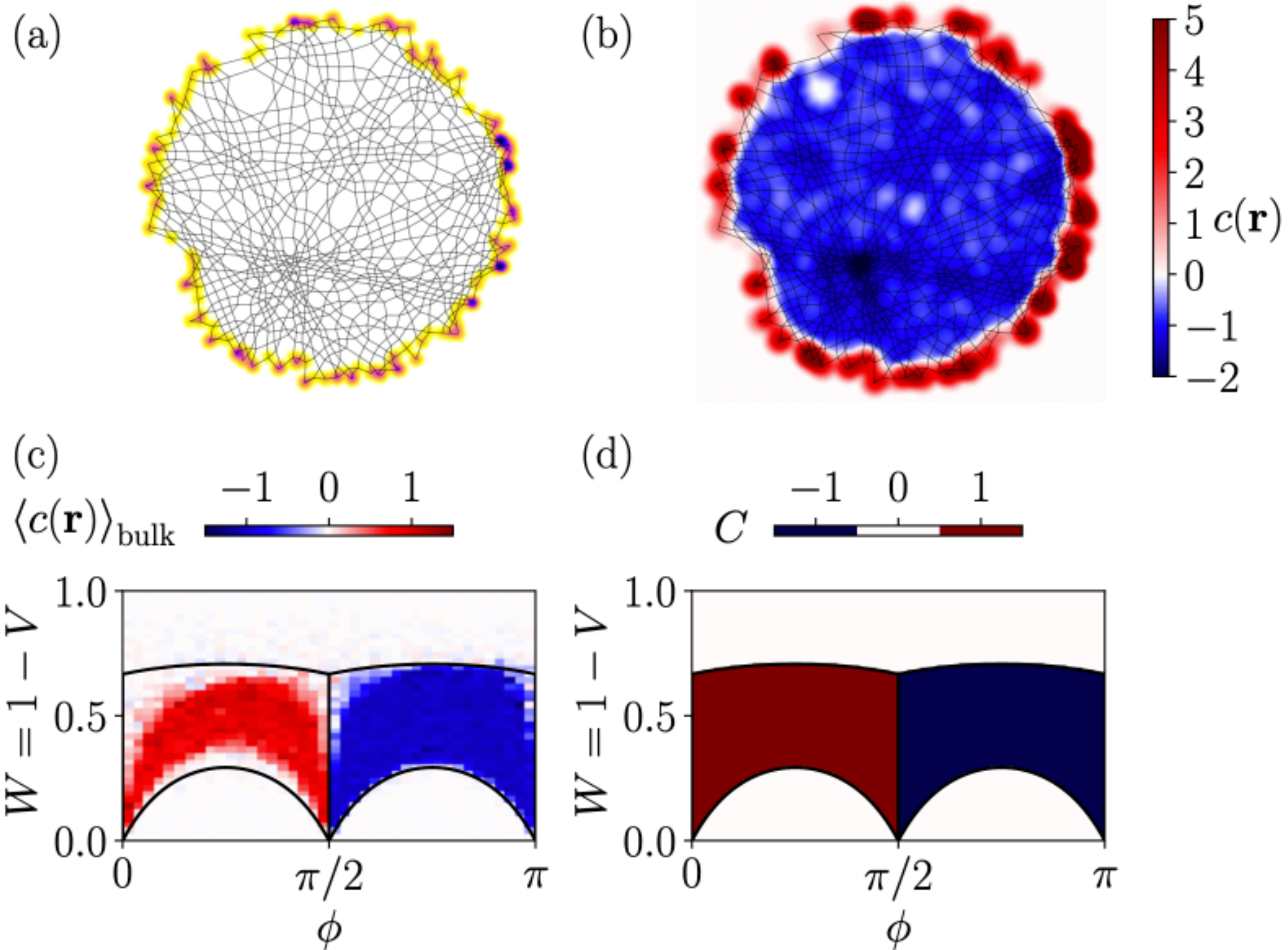
# Topological Weaire-Thorpe model

Q. N



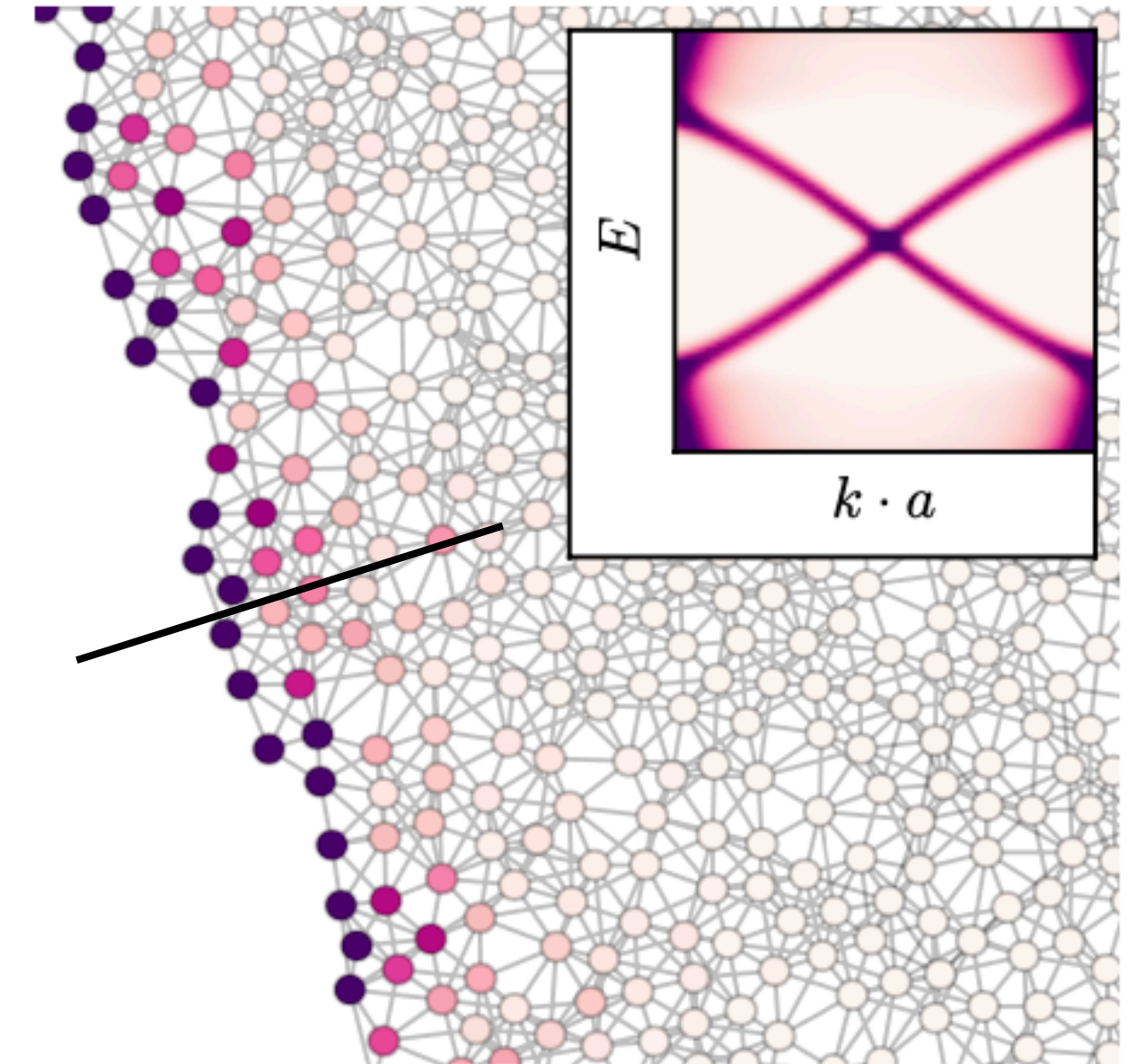
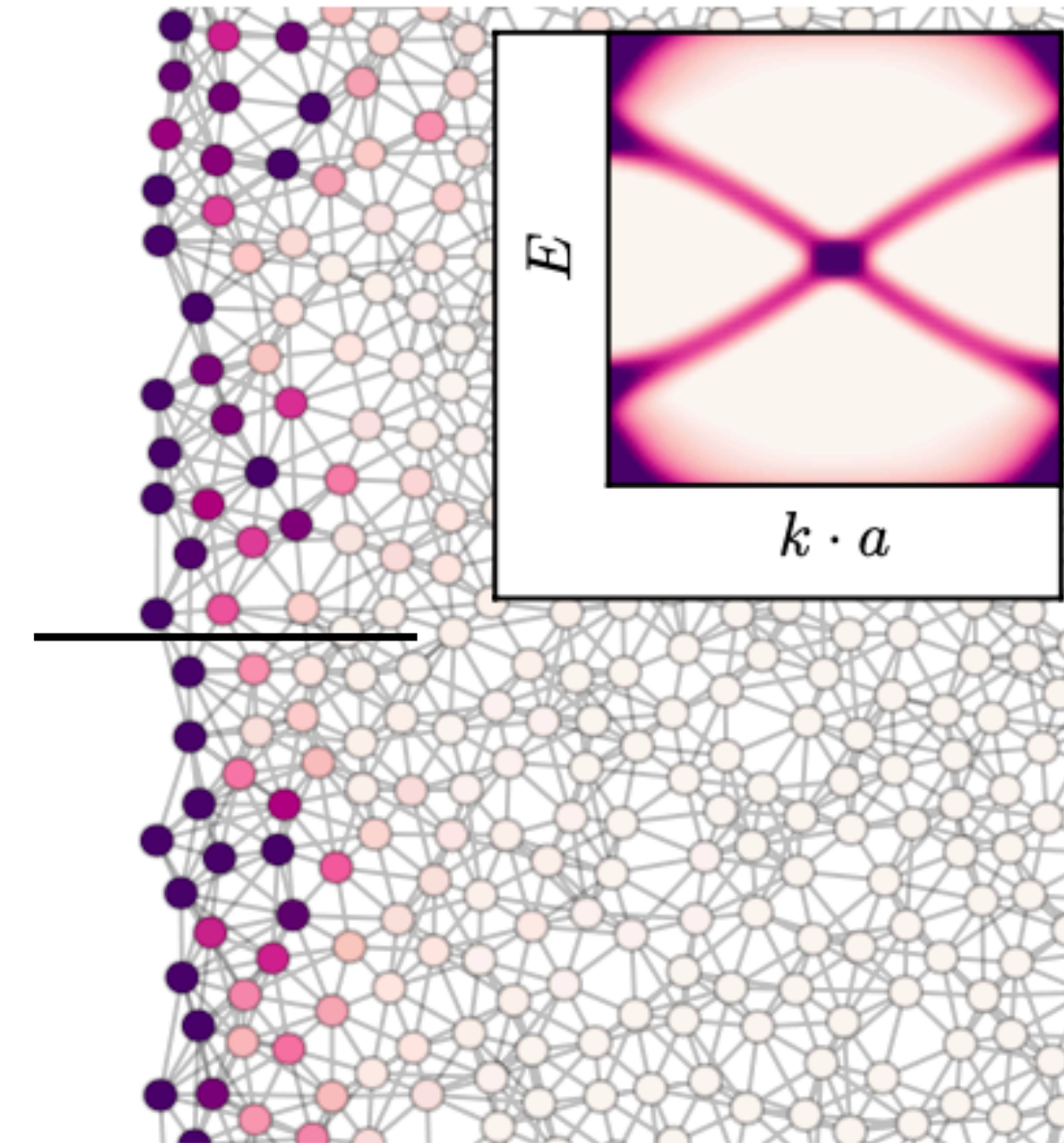
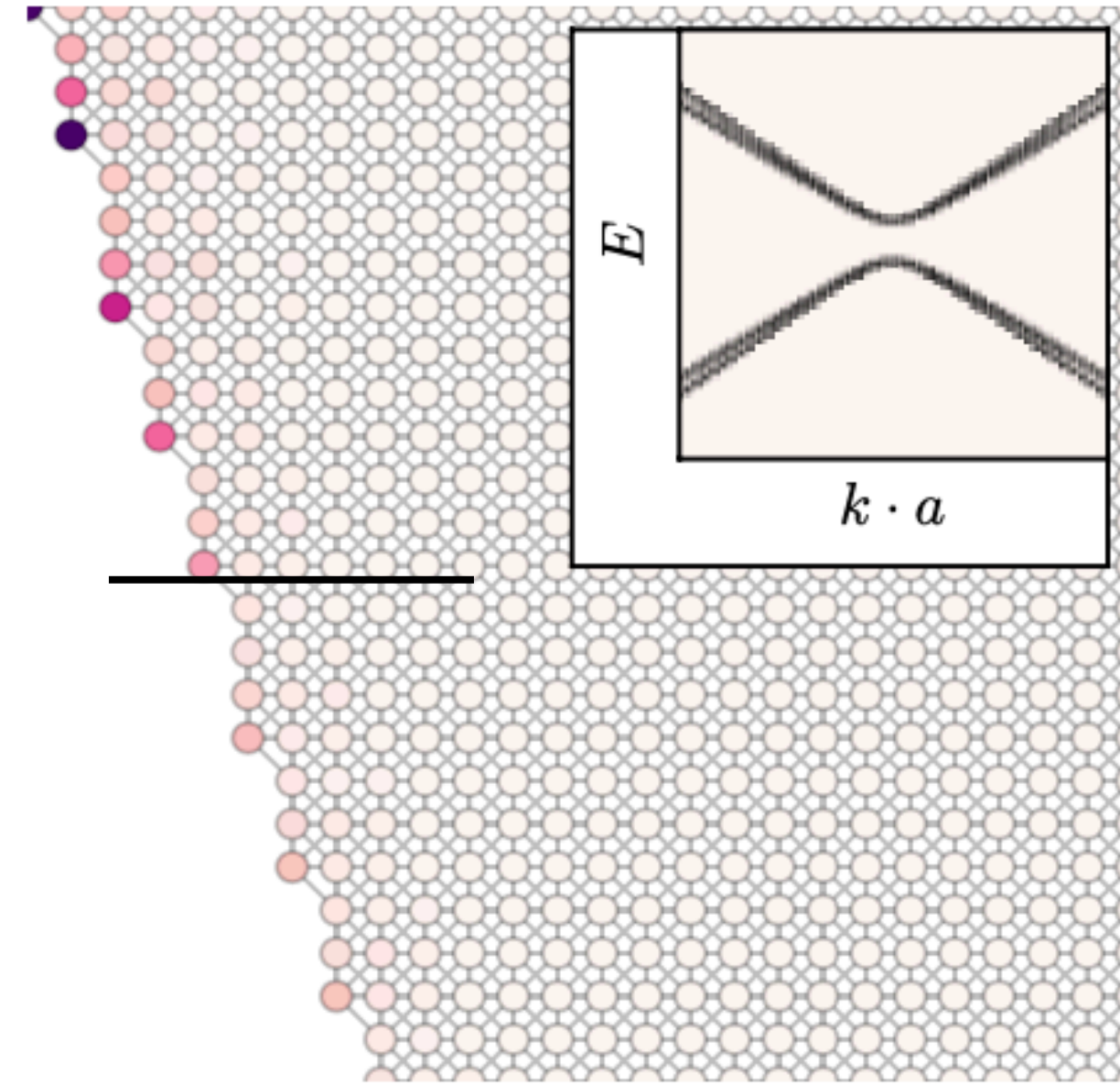
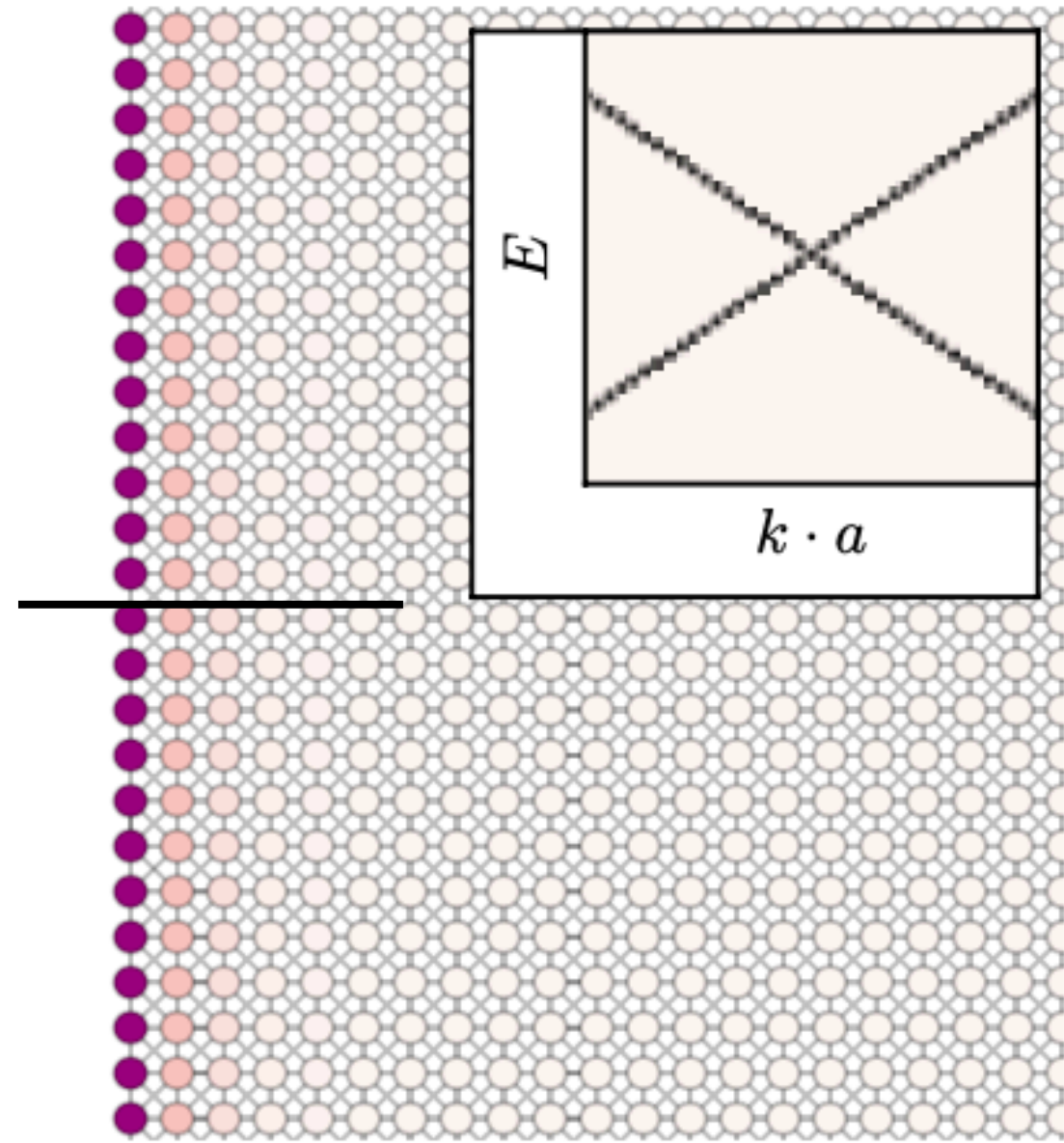
Que  
Néel





# Average symmetries — enhanced robustness

Spring, Akhmerov, Varjas Sci. Post (2020)



Mirror preserved

robust edge state



Broken mirror

no edge state



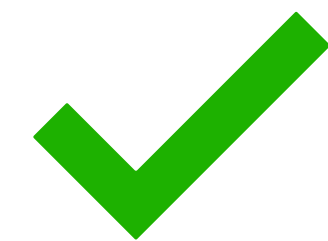
Mirror preserved  
on average

robust edge state



Mirror preserved  
on average

robust edge state



# Technical details I

Spectral weight:

$$F_{\pm}(|\psi\rangle) = \sum_j |\langle j, \pm | \psi \rangle|^2$$

$$F_m(|\psi\rangle) = \sum_i |\langle i, m | \psi \rangle|^2$$

$$F_m(E) = \frac{1}{N} \text{Tr} \left[ \delta(H - E) \hat{F}_m \right]$$

Hamiltonian

$$H = \sum_{i,j \neq j'}^z V_{jj'}^{(i)} |i, j\rangle \langle i, j'| + \sum_{i \neq i', j}^z W_{ii'}^{(j)} |i, j\rangle \langle i', j|.$$

$$H_V |i, m\rangle = 2V \cos \left( \phi + m \frac{2\pi}{3} \right) |i, m\rangle \equiv \lambda_m |i, m\rangle,$$

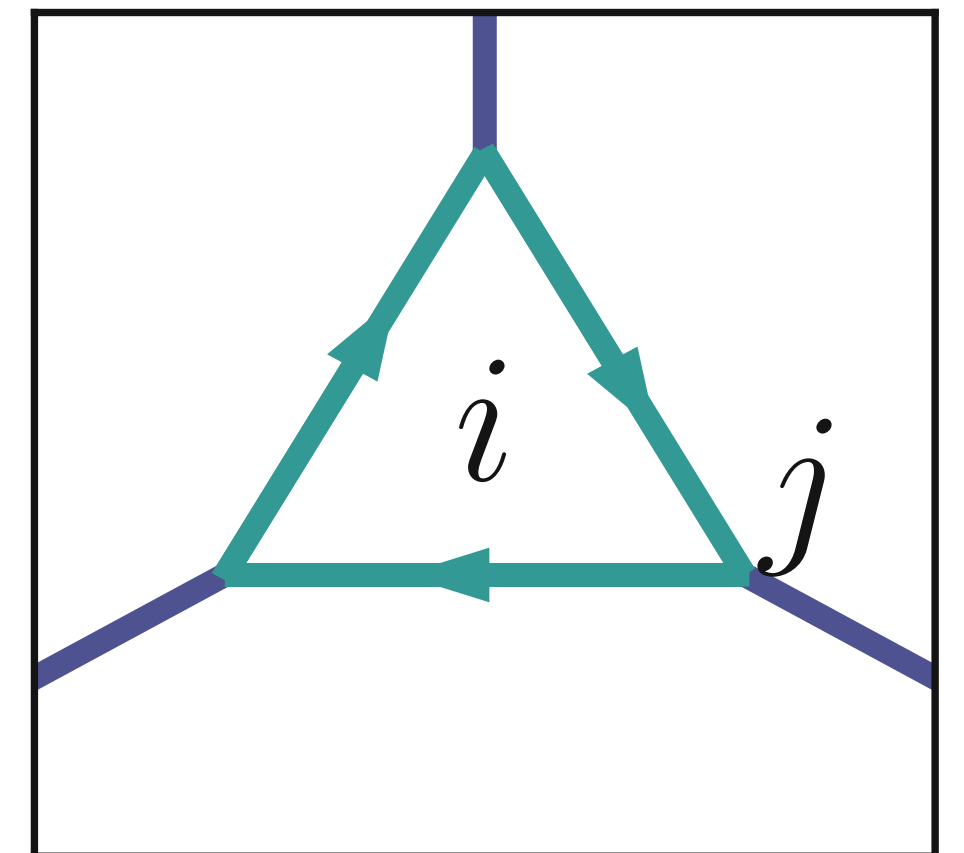
$$R |i, m\rangle = e^{i \frac{2m\pi}{3}} |i, m\rangle \equiv \xi_m |i, m\rangle.$$

$$H_W |j, \pm\rangle = \pm W |j, \pm\rangle,$$

$$I |j, \pm\rangle = \pm |j, \pm\rangle.$$

$$H_V = V \begin{pmatrix} 0 & e^{i\phi} & e^{-i\phi} \\ e^{-i\phi} & 0 & e^{i\phi} \\ e^{i\phi} & e^{-i\phi} & 0 \end{pmatrix}$$

$$\mathcal{C}(\mathbf{r}) = 2\pi \text{Im} \langle \mathbf{r} | [\hat{Q}\hat{x}, \hat{P}\hat{y}] | \mathbf{r} \rangle$$



# Mapping to continuous media: effective Hamiltonian

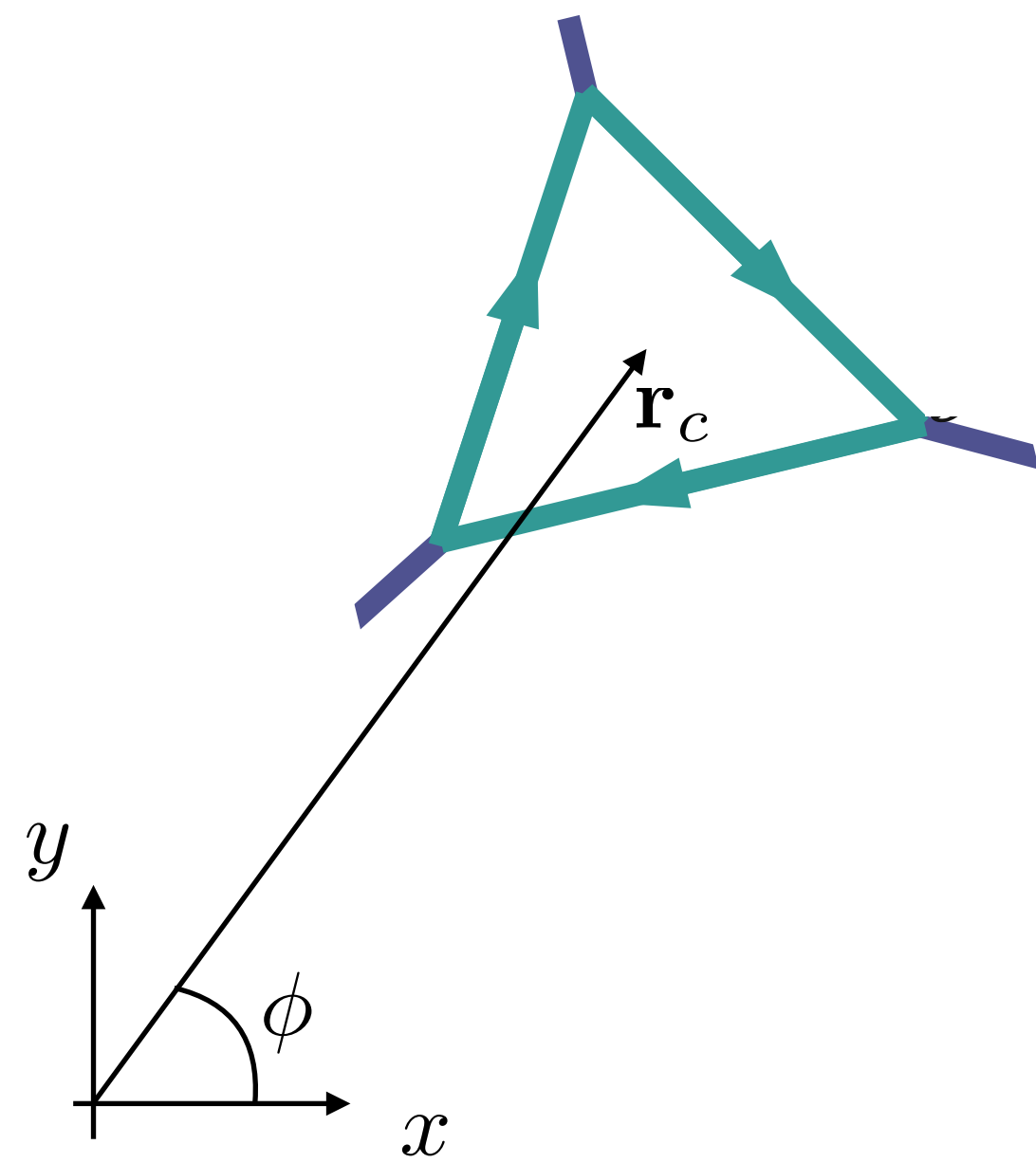
Q. Marsal, D. Varjas, AGG PNAS, (2020)

$$G_l(\mathbf{k}) = \langle \mathbf{k}l | H | \mathbf{k}l \rangle$$

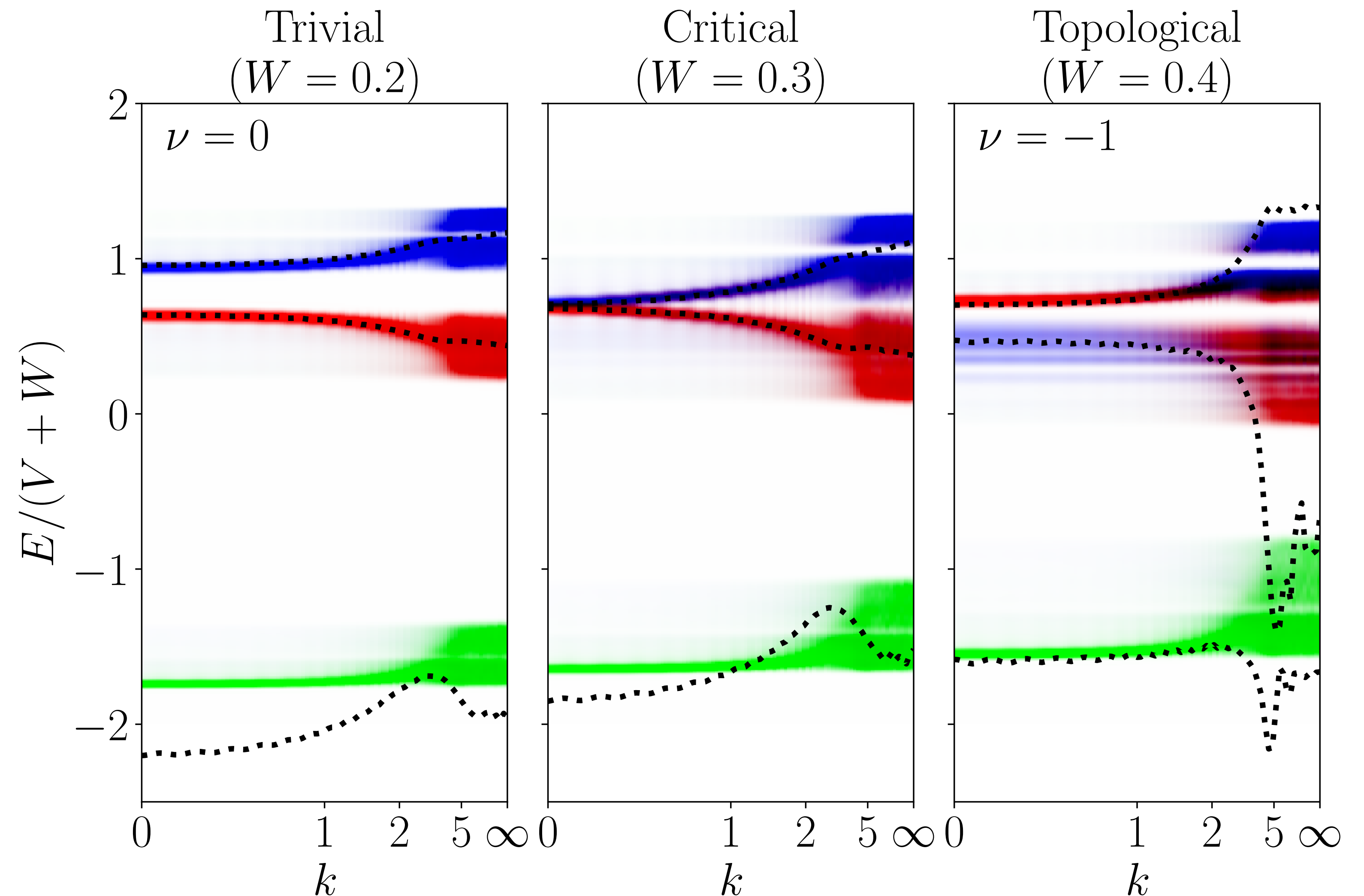
Varjas et al. PRL (2020)

$$\langle \mathbf{r} | \mathbf{k}, l \rangle = \frac{1}{\sqrt{N}} \exp(i\mathbf{k}\mathbf{r}_c) \exp(i\phi_{\mathbf{r}}l),$$

$$H_{\text{eff}}(\mathbf{k}) = G_l^{-1}(\mathbf{k}) - E_F$$



$$\nu = \sum_n l_n(|\mathbf{k}| = 0) - l_n(|\mathbf{k}| = \infty)$$



Q. Marsal, D. Varjas, AGG PNAS (2020)

Technical details: Structural spillage

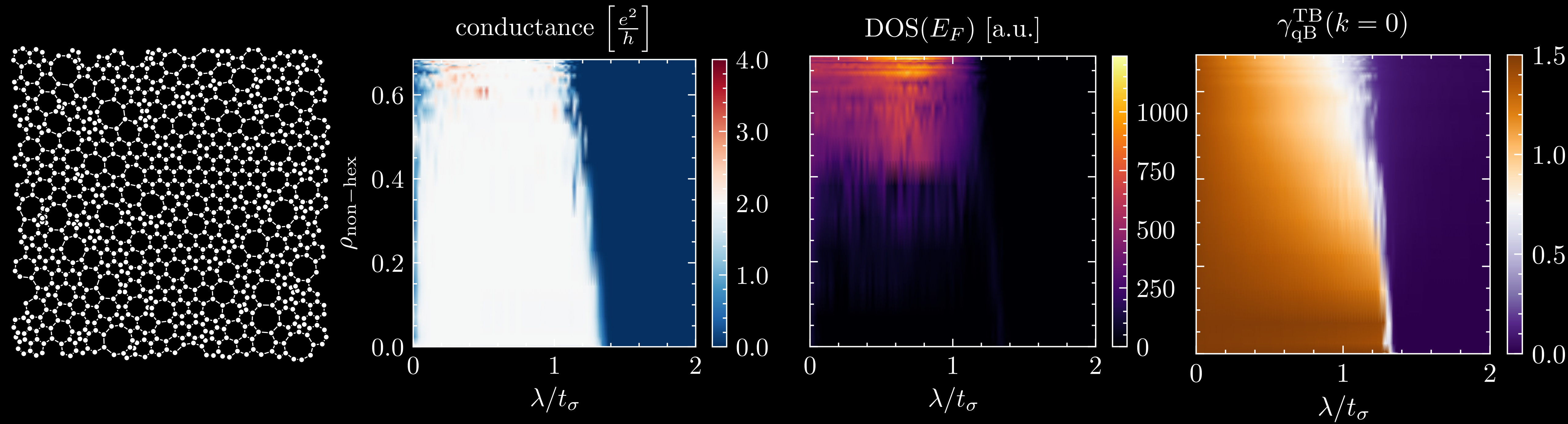
## Structural spillage TB

problem = plane waves not well defined in all space

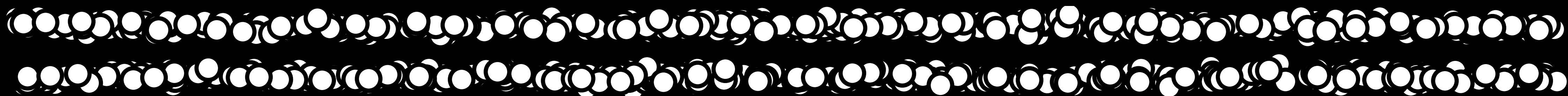
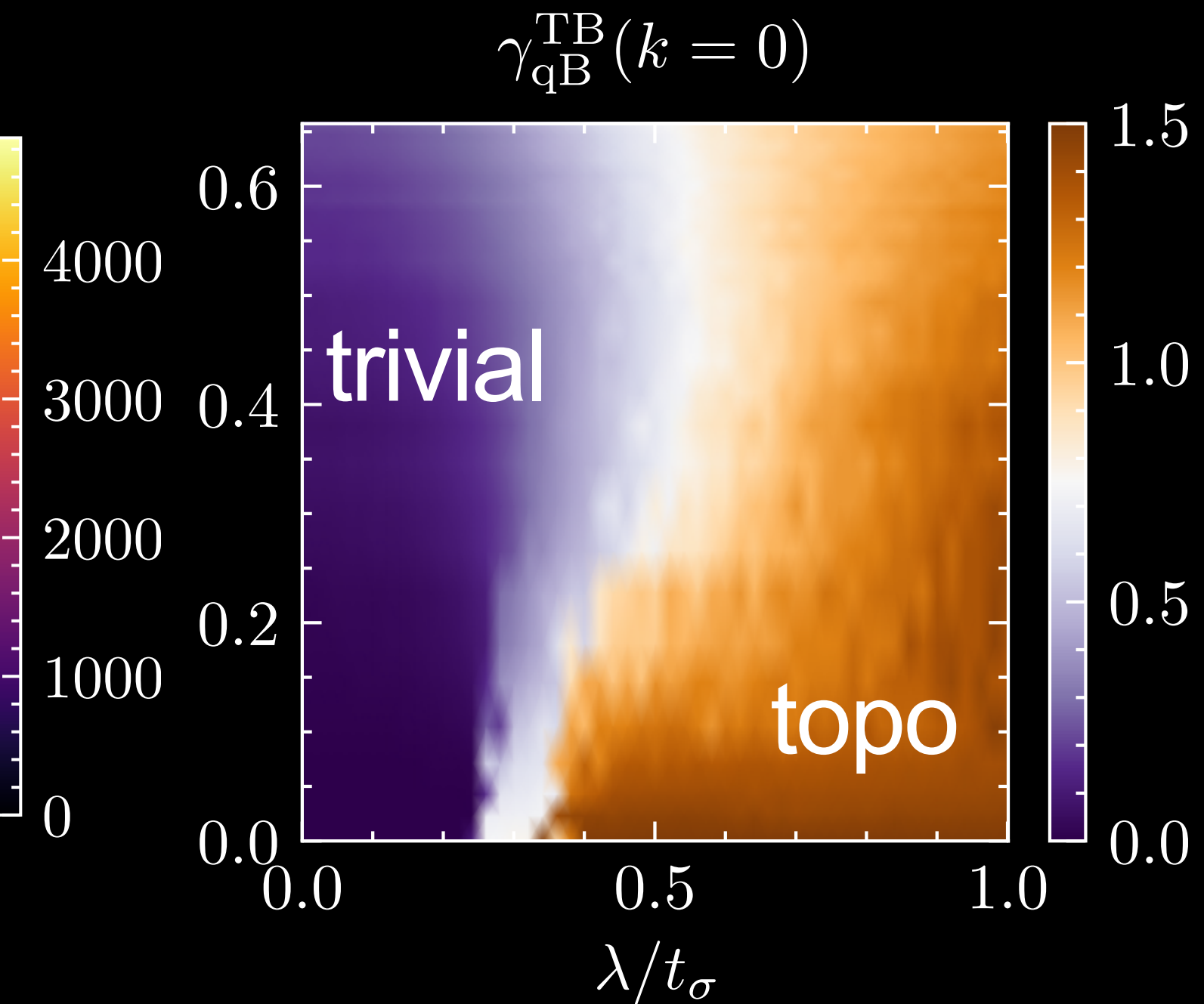
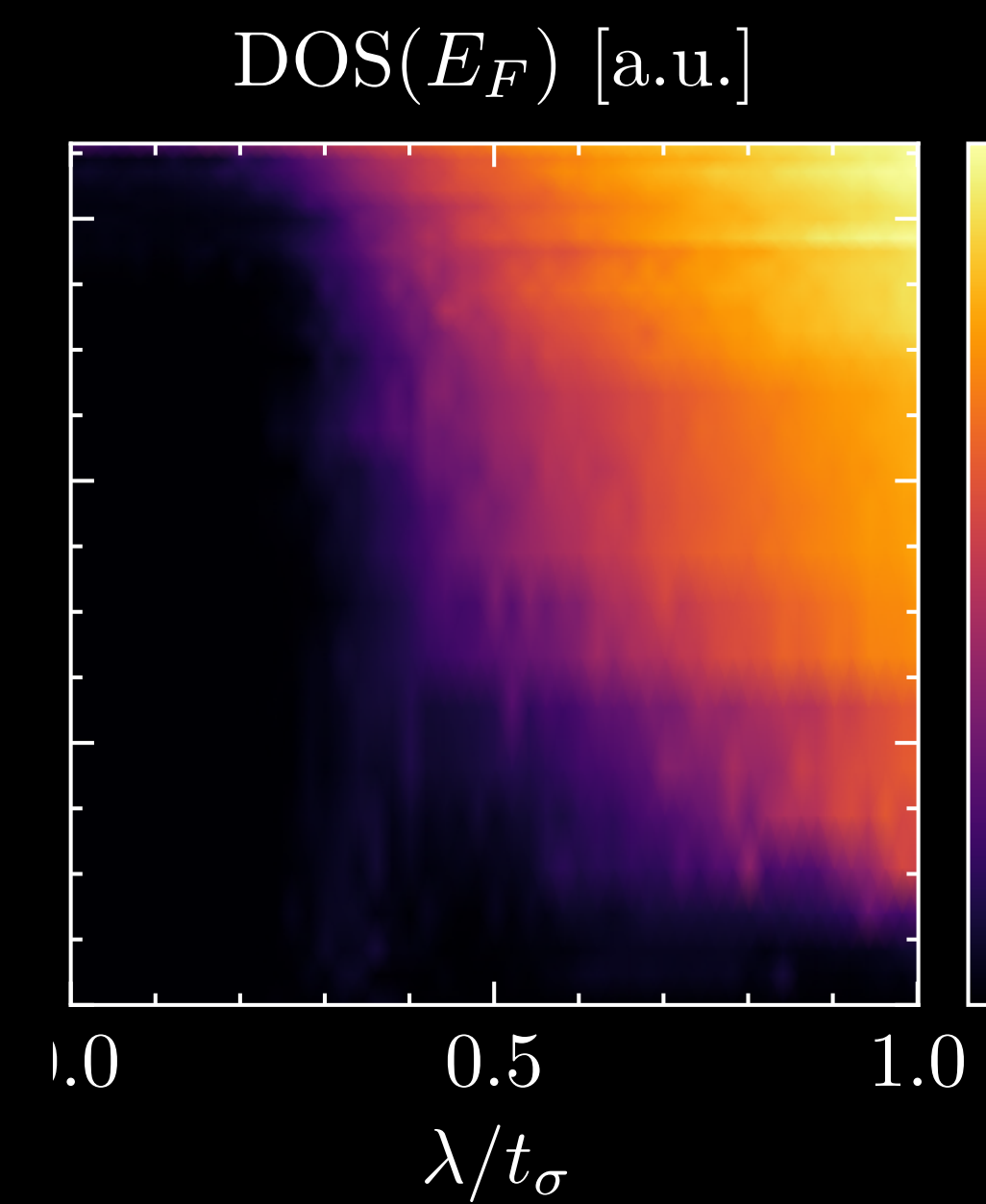
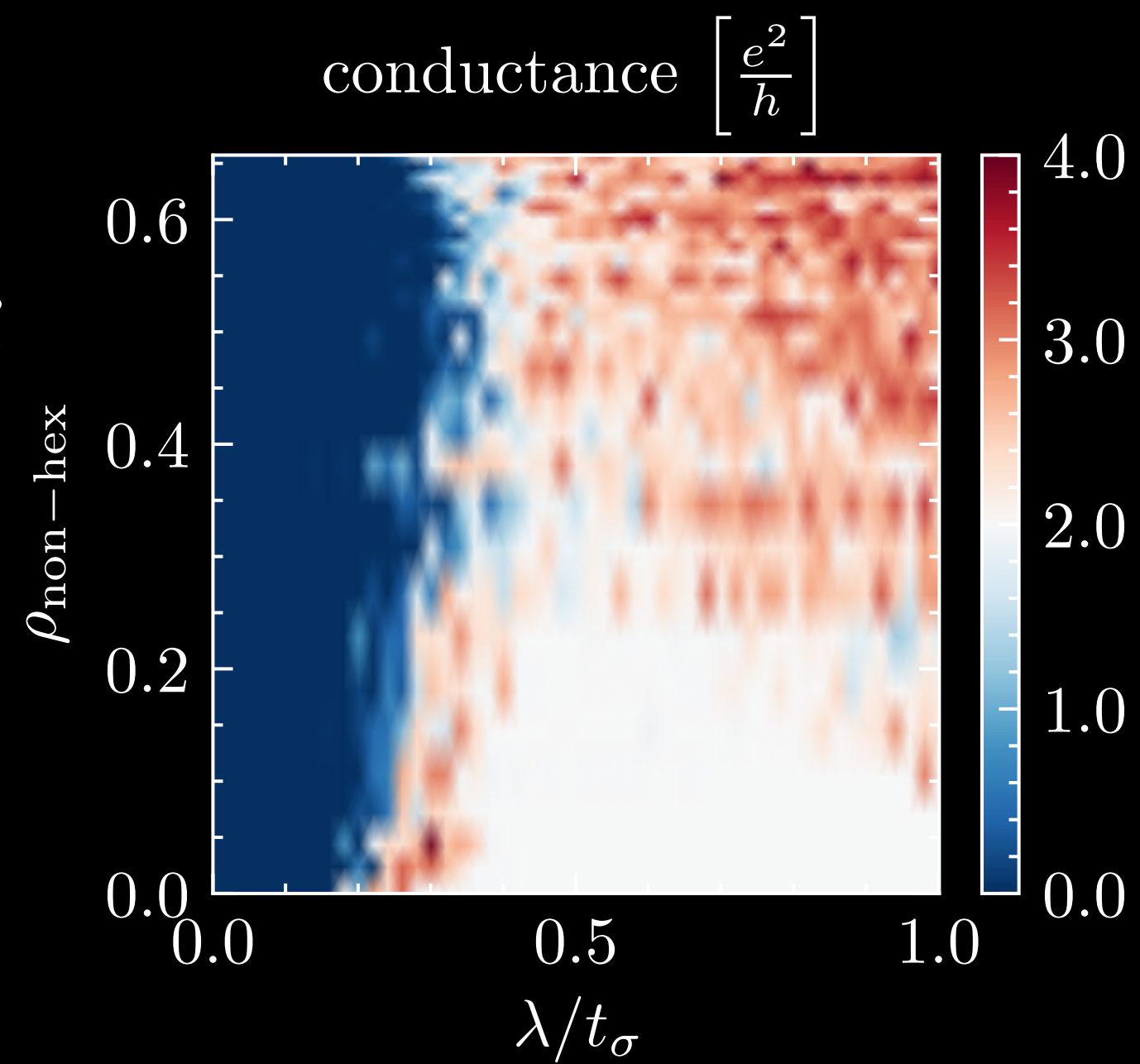
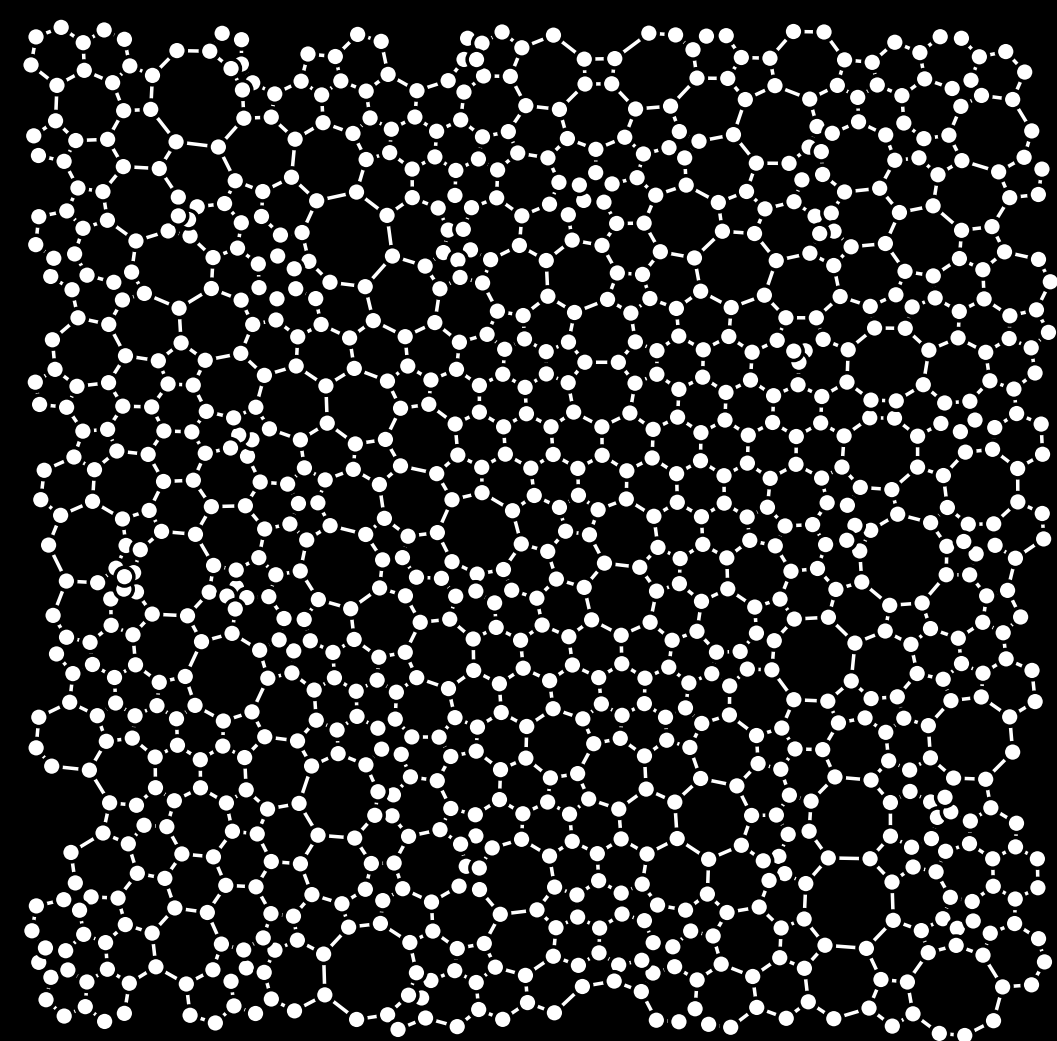
problem = different BZs

$$\gamma_{\text{qB}}^{\text{TB}}(\mathbf{k}) = \frac{1}{2} \frac{N_{\text{s/c}}}{N_{\text{BZs}}} \sum_{\mathbf{G} \in \text{BZs}} \text{tr} \left[ \left( P_{\mathbf{k}+\mathbf{G}} - \tilde{P}_{\mathbf{k}+\mathbf{G}} \right)^2 \right]$$

# Tight-binding bismuthene



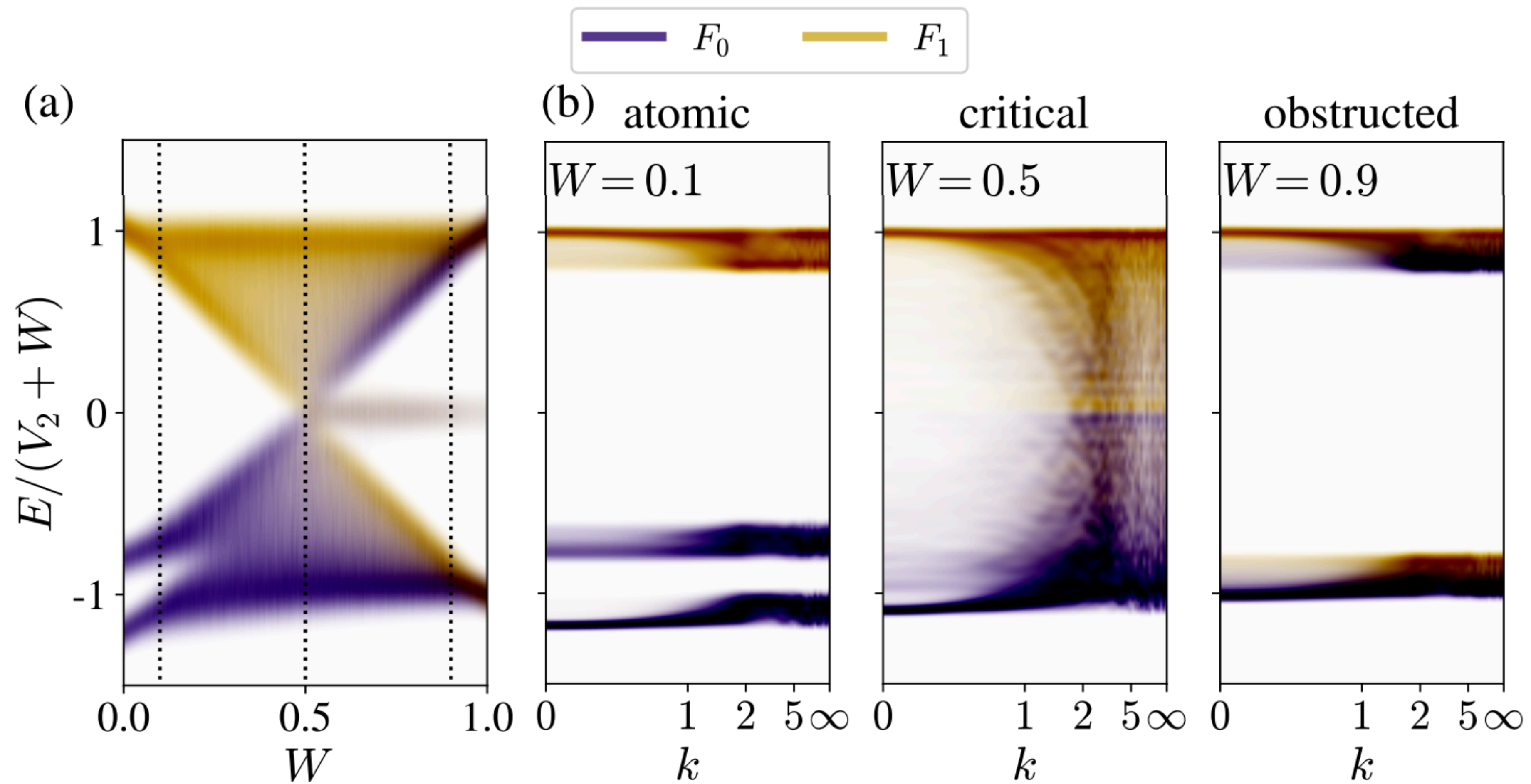
# Tight-binding bismuth bilayer

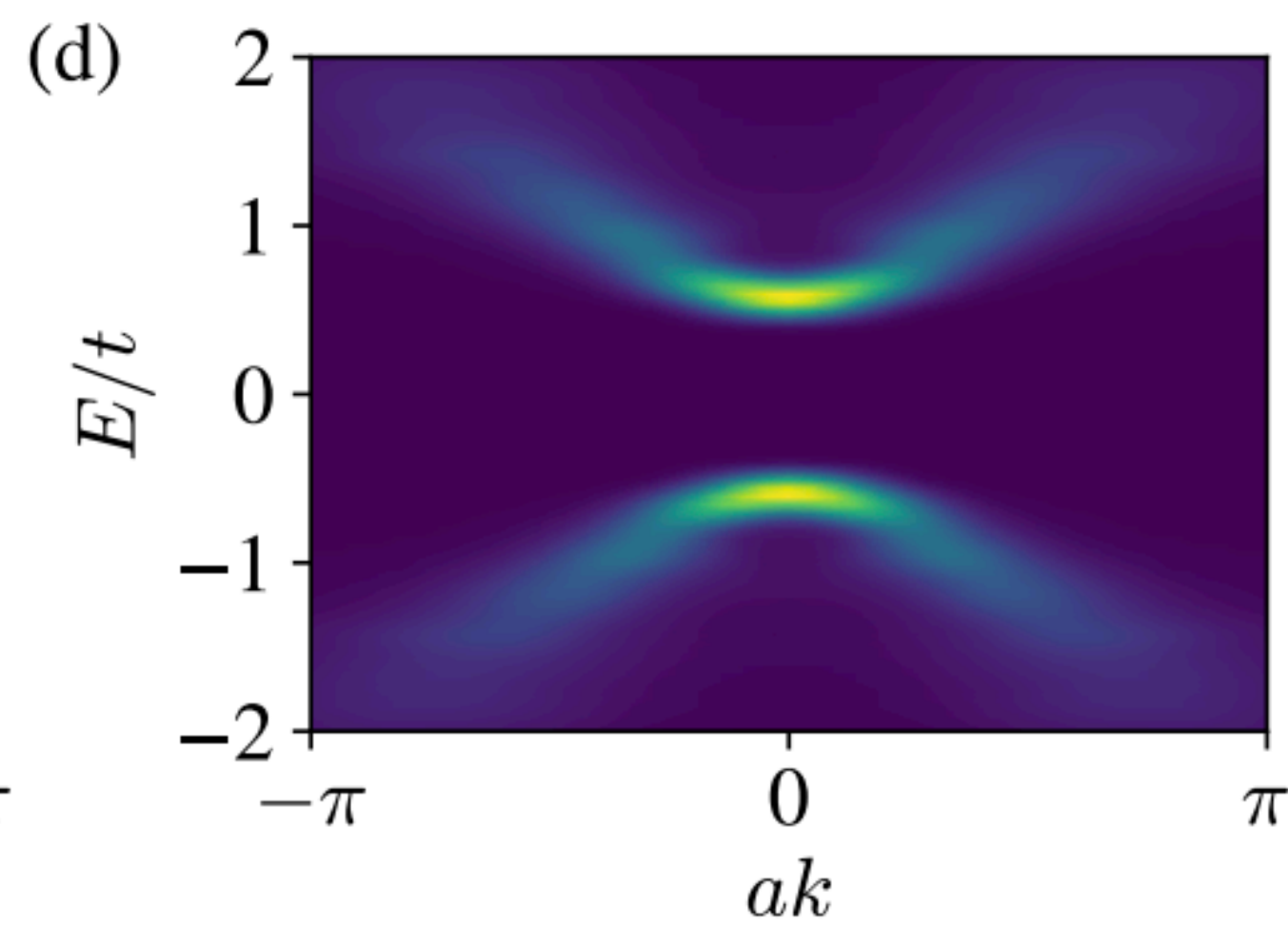
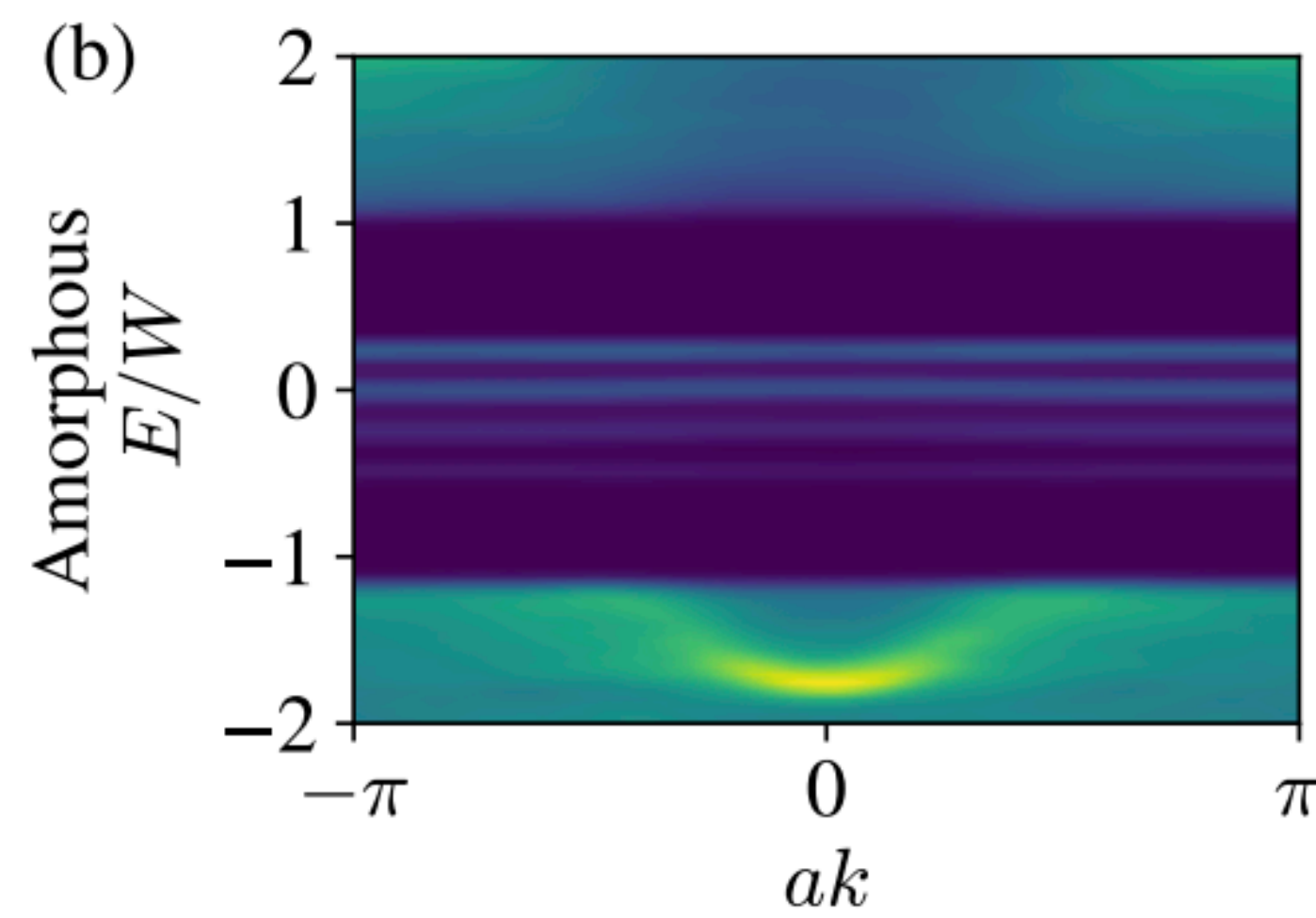
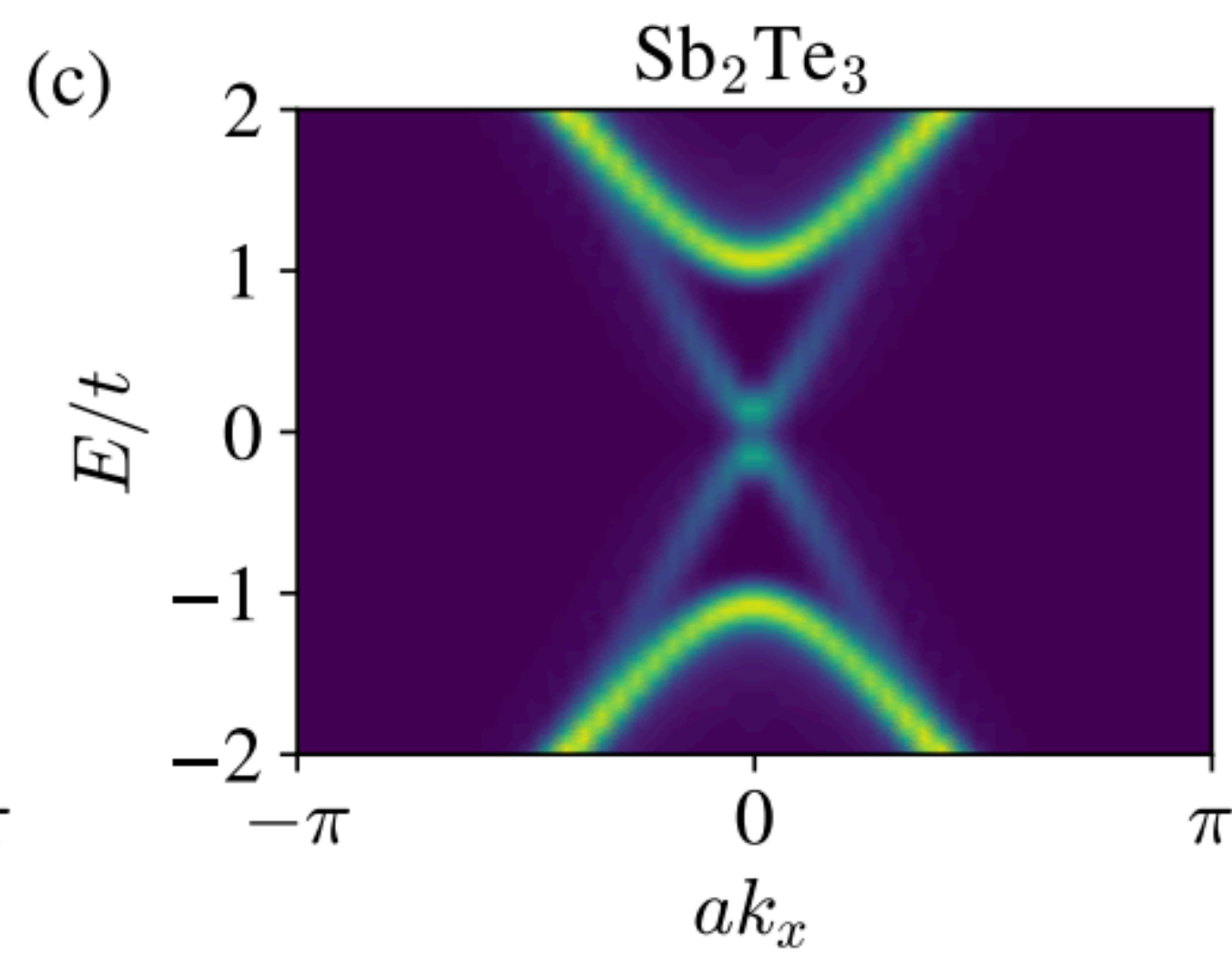
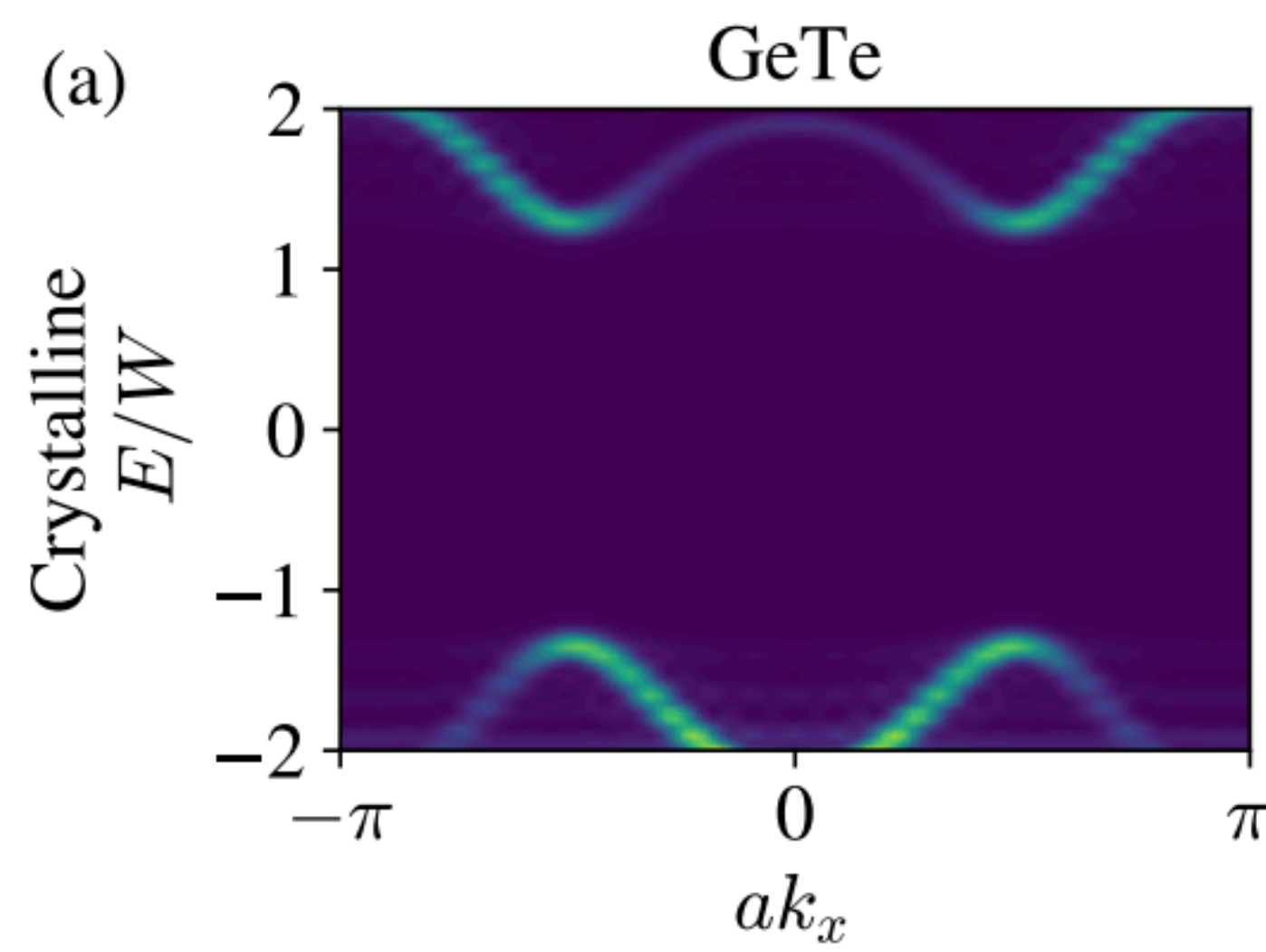






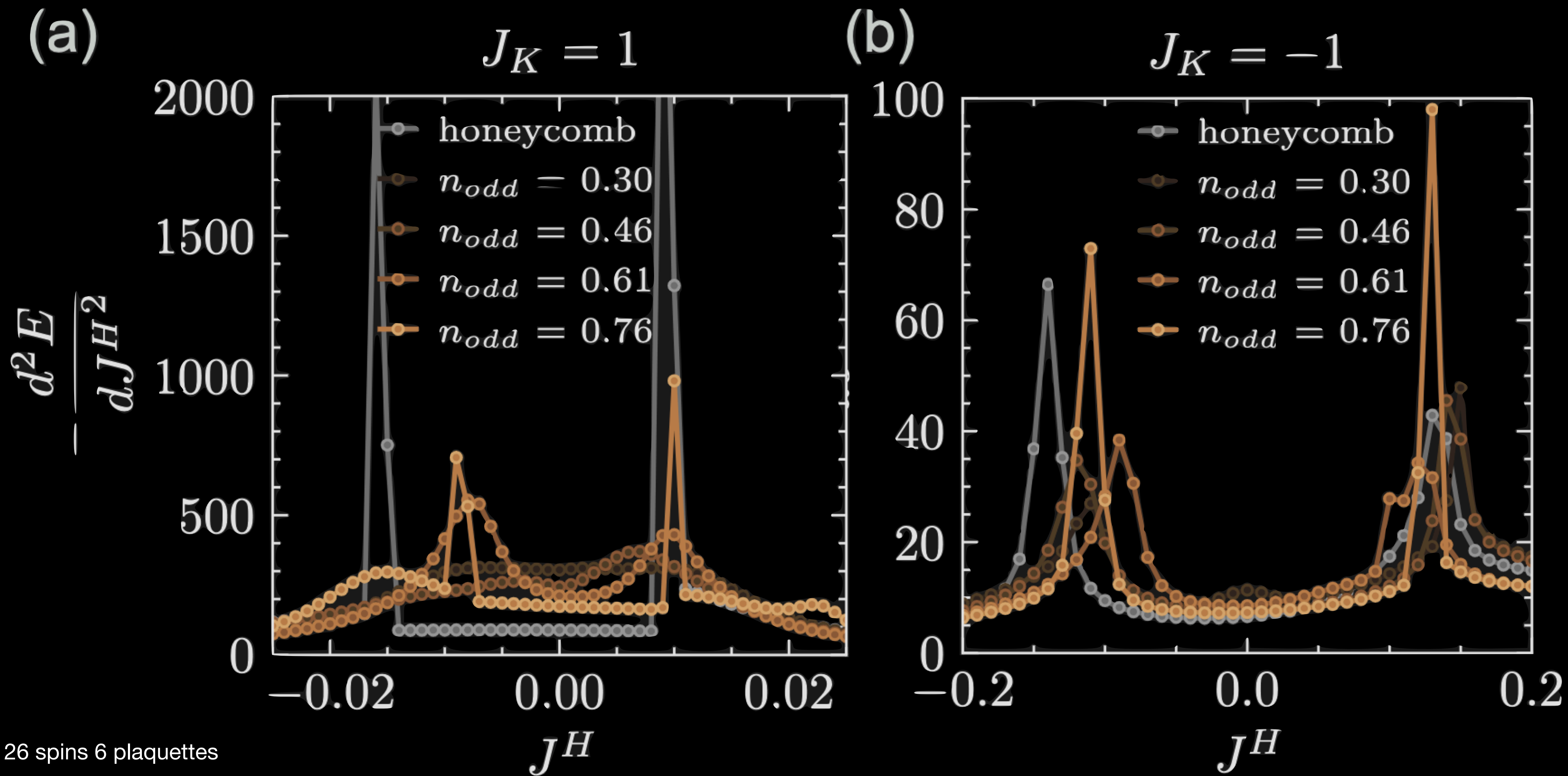
Technical details: Obstructed / phase change





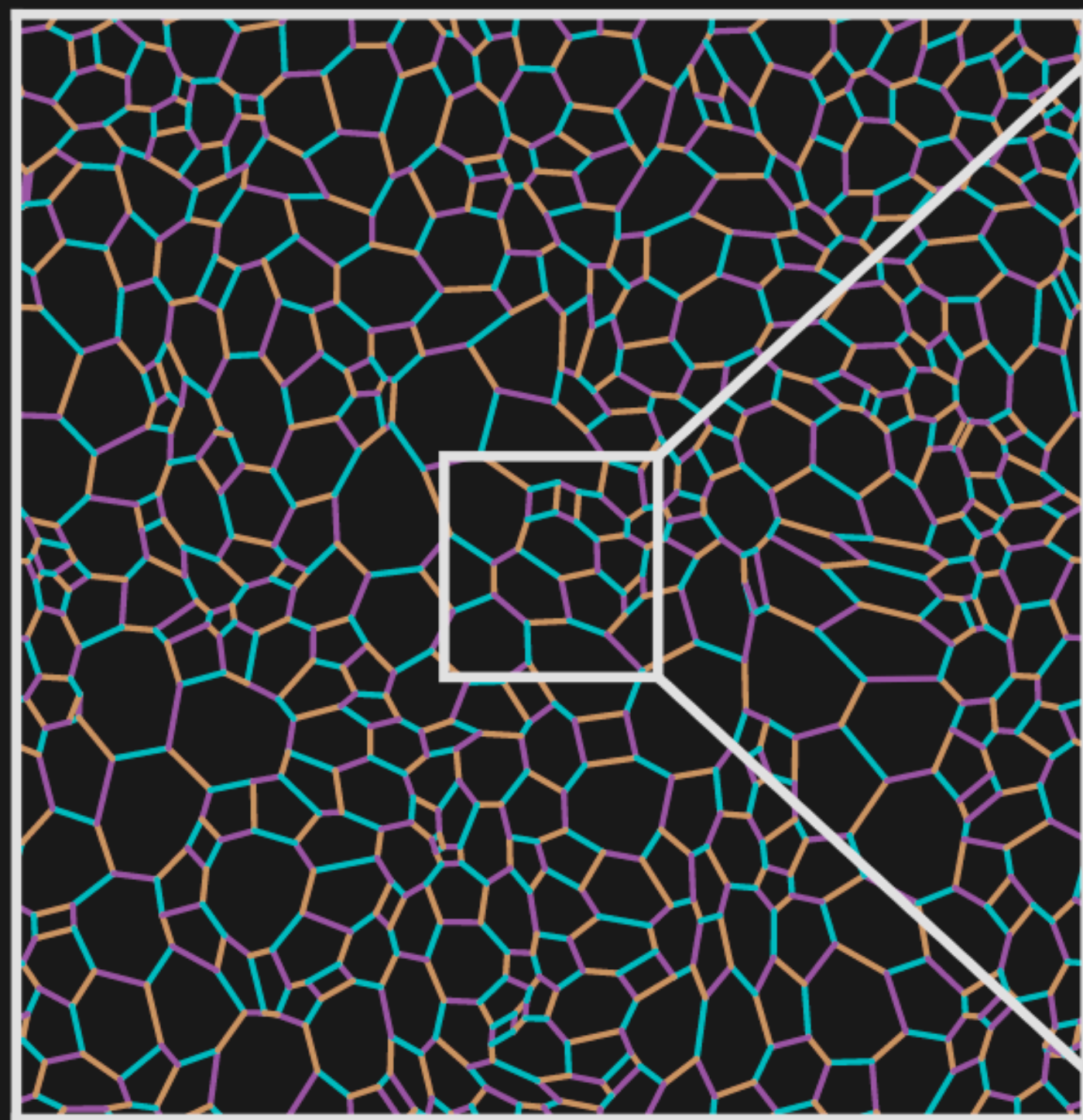
$$H = \sum_i V(\mathbf{c}_i^\dagger \wedge \mathbf{c}_i) \cdot \mathbf{S} + (-1)^i \epsilon \mathbf{c}_i^\dagger \cdot \mathbf{c}_i - \sum_{\langle i,j \rangle} (W + (-1)^i \text{sgn}(\hat{d}_{ij} \cdot (\hat{e}_x + \hat{e}_y + \hat{e}_z) \Delta W)) (\mathbf{c}_i^\dagger \cdot \hat{d}_{ij}) (\mathbf{c}_j \cdot \hat{d}_{ji}),$$

Technical details: amorphous Kitaev

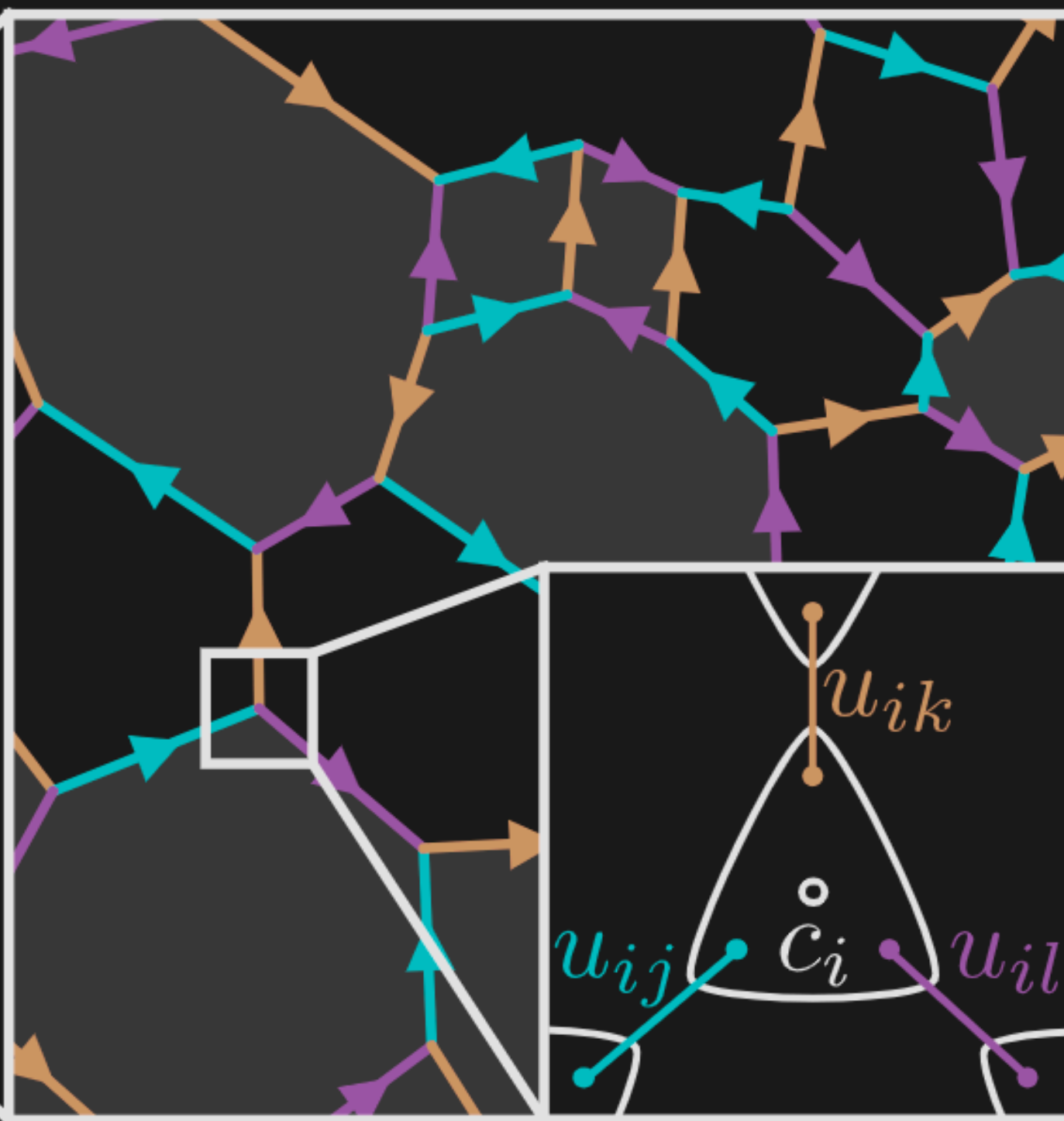


$$H_{kh} = J^K \sum_{i,k,\alpha} \sigma_j^\alpha \sigma_k^\alpha + J^H \sum_{\langle ij \rangle} \sigma_i \cdot \sigma_j.$$

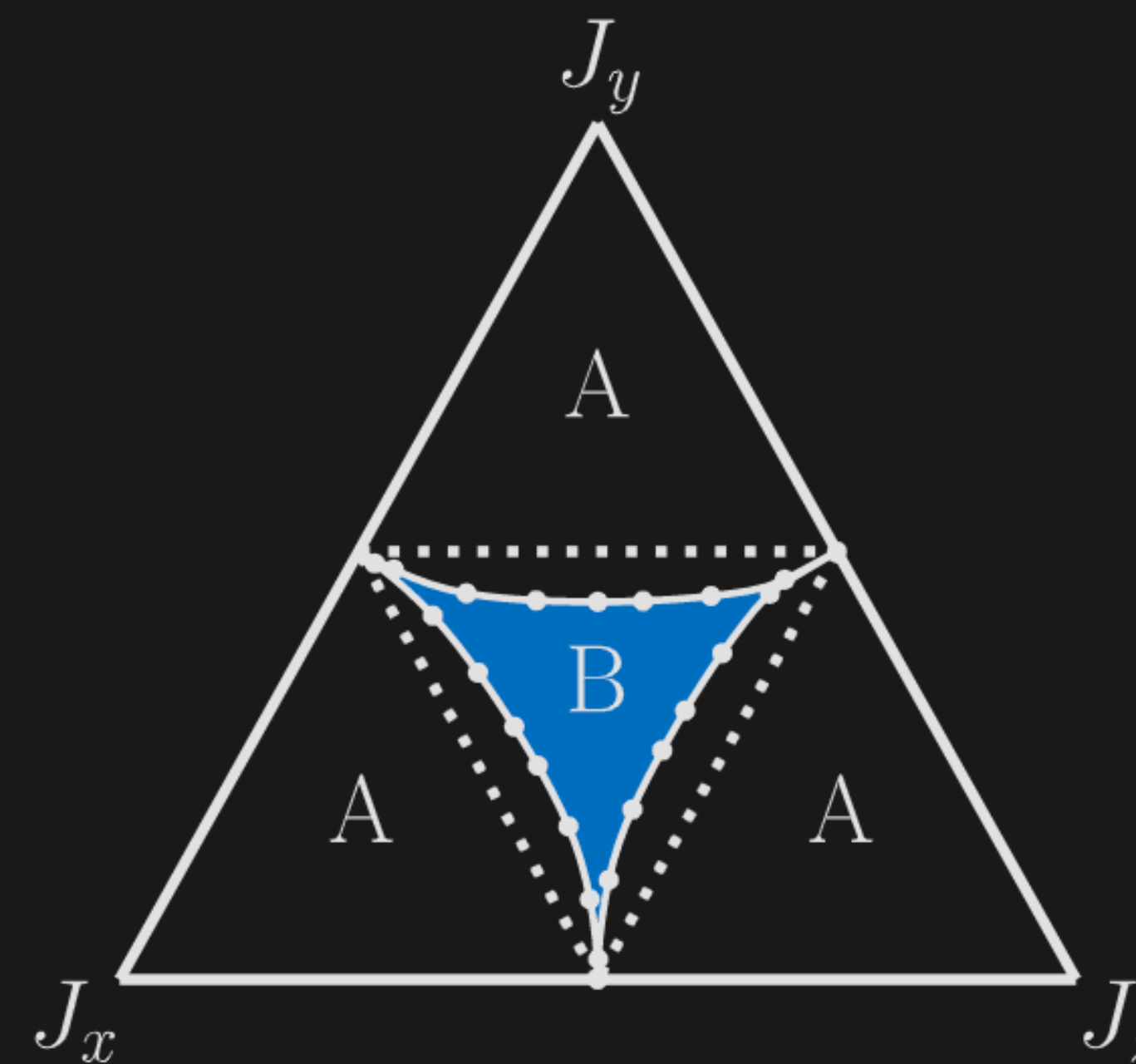
(a)



(b)



(c)



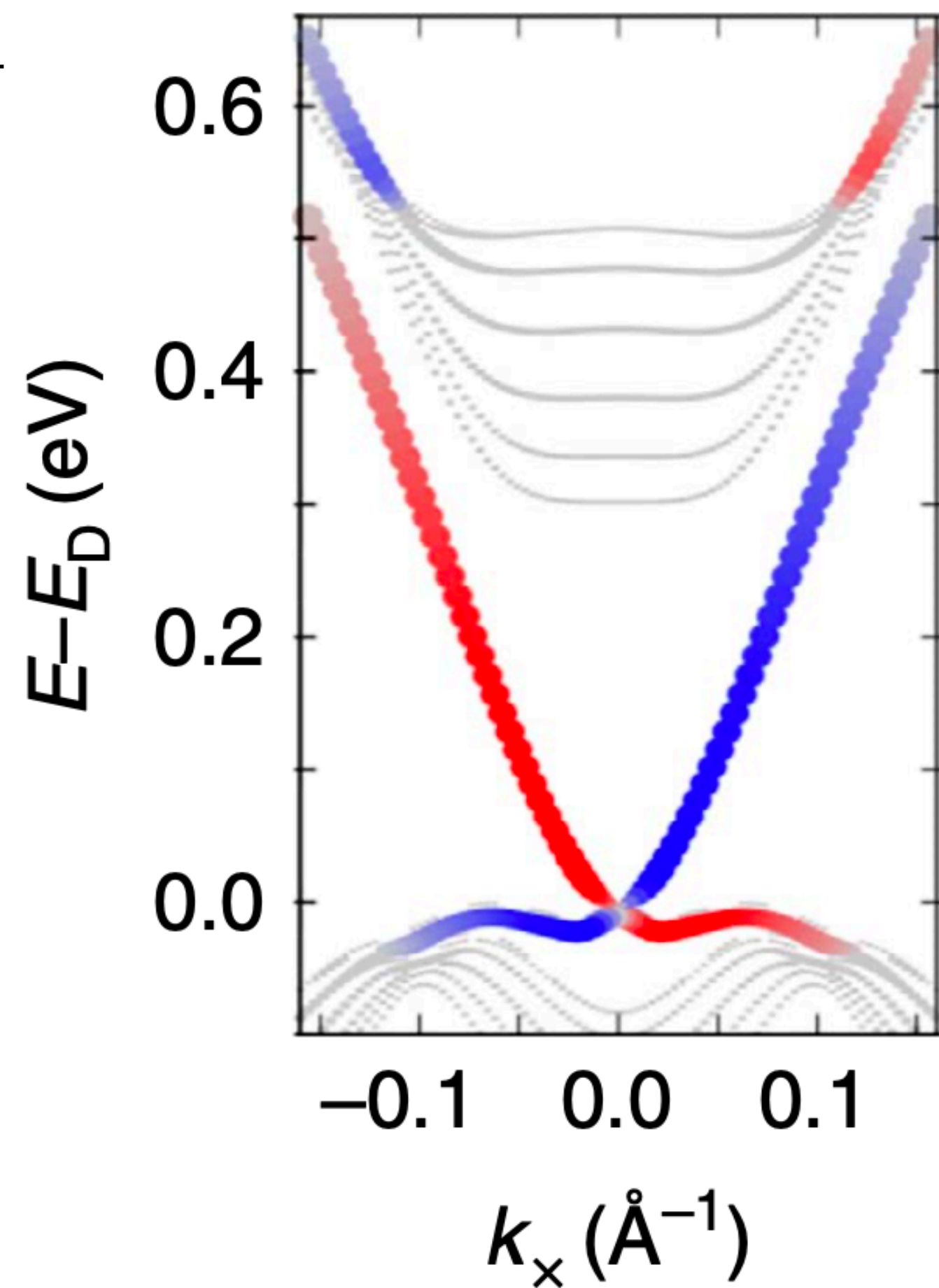


Technical details: amorphous  $\text{Bi}_2\text{Se}_3$

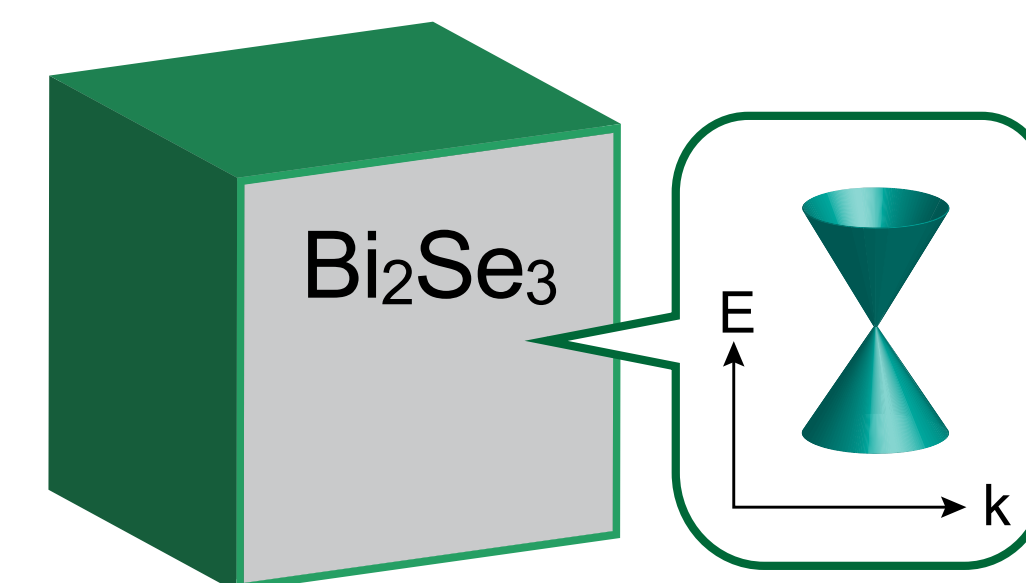
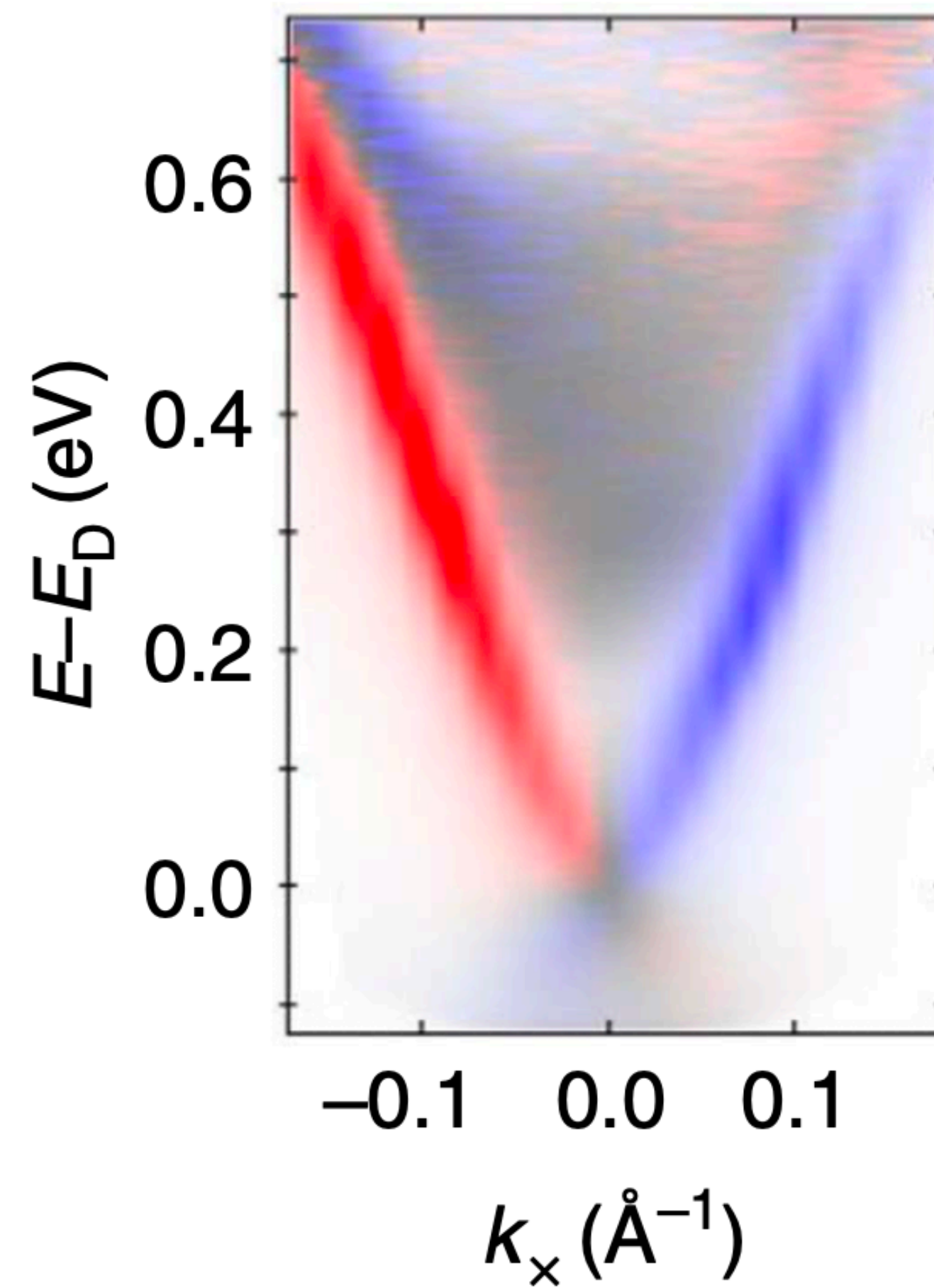
# A textbook example of a 3D-topological insulator

## $\text{Bi}_2\text{Se}_3$

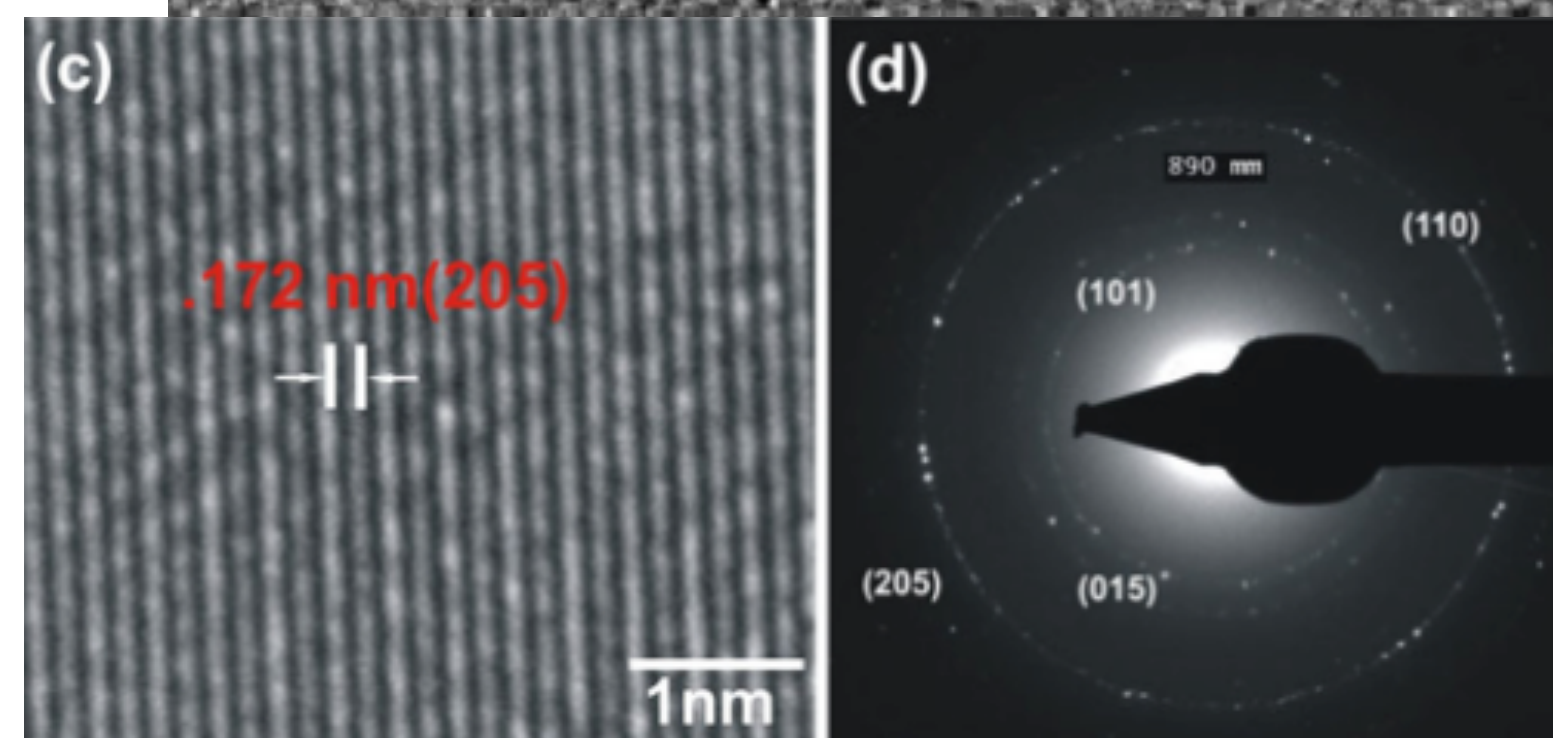
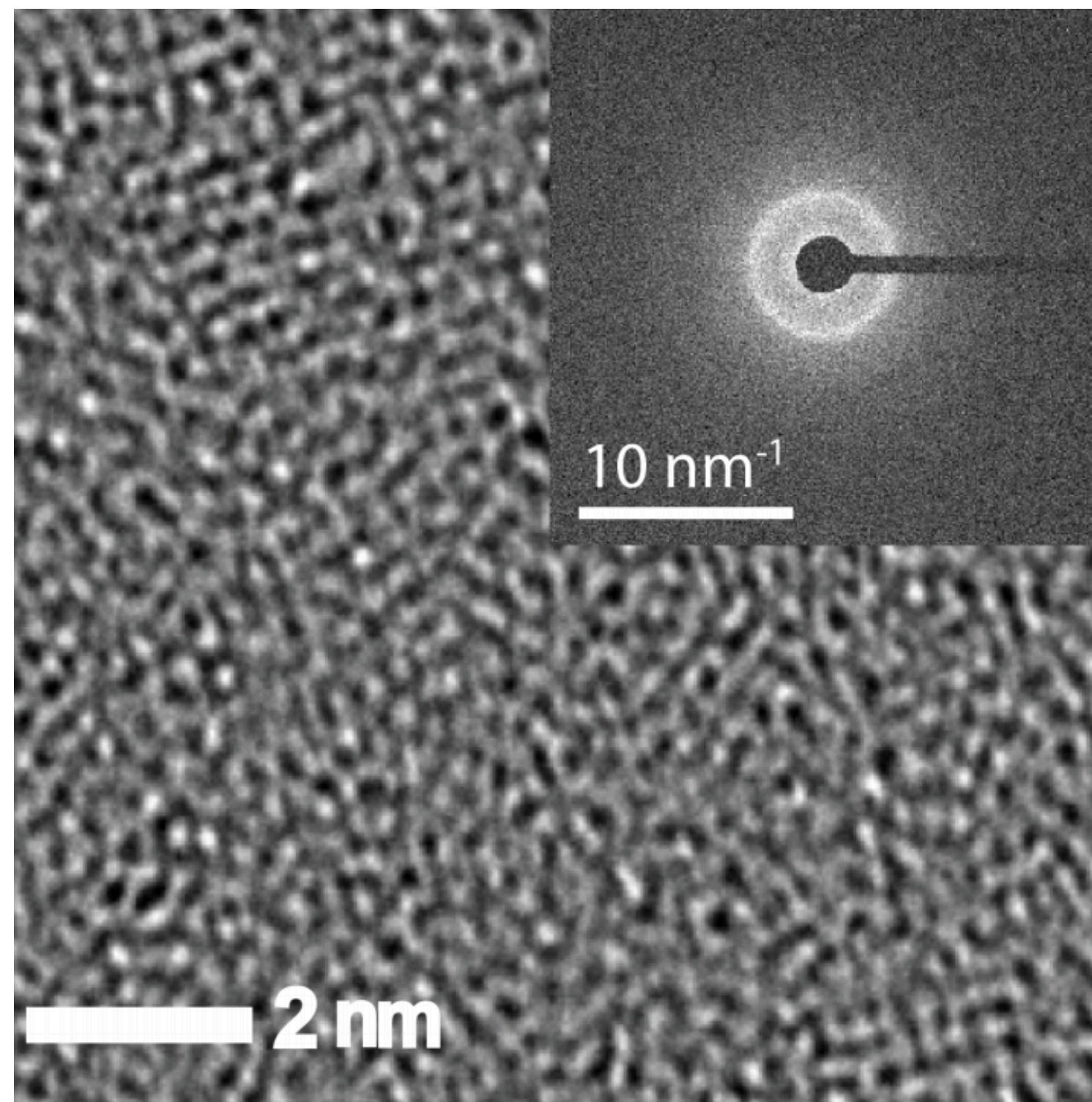
DFT



ARPES



# Amorphous $\text{Bi}_2\text{Se}_3$

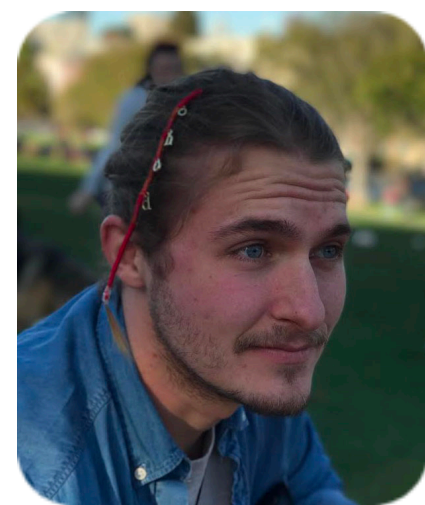


5 nm



Paul Corbae

(Hellman group, UCB)



Sam Ciocys

(Lanzara group, LBL)

Kadel et al. *Nanoscale Res. Lett.* (2011)

[see also J. Barzola-Quiquia, et al. *Journal of Applied Physics* (2015)]

# Amorphous $\text{Bi}_2\text{Se}_3$

Transport

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ARPES

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spin resolved ARPES

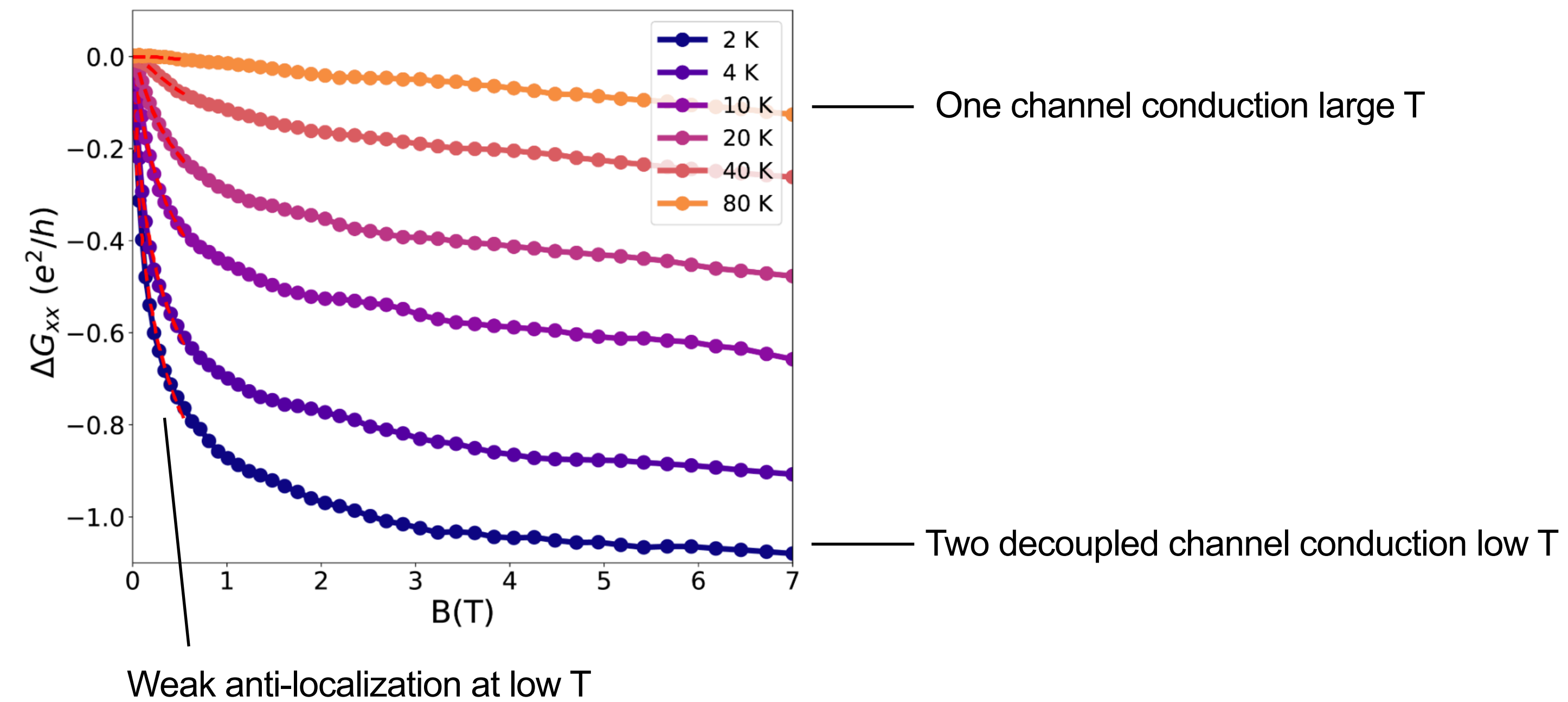
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# Amorphous $\text{Bi}_2\text{Se}_3$

## Transport

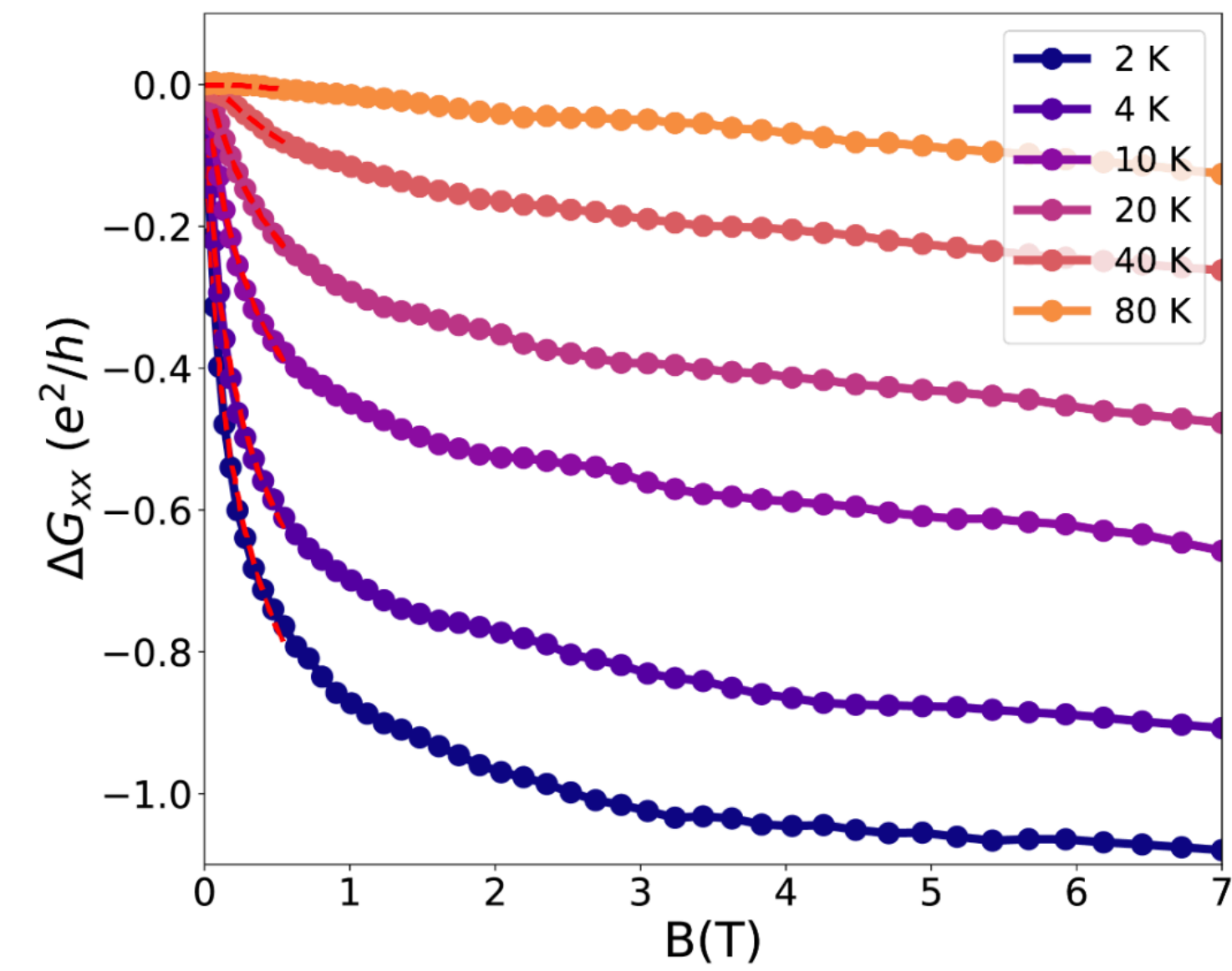
## ARPES

## spin resolved ARPES



# Amorphous $\text{Bi}_2\text{Se}_3$

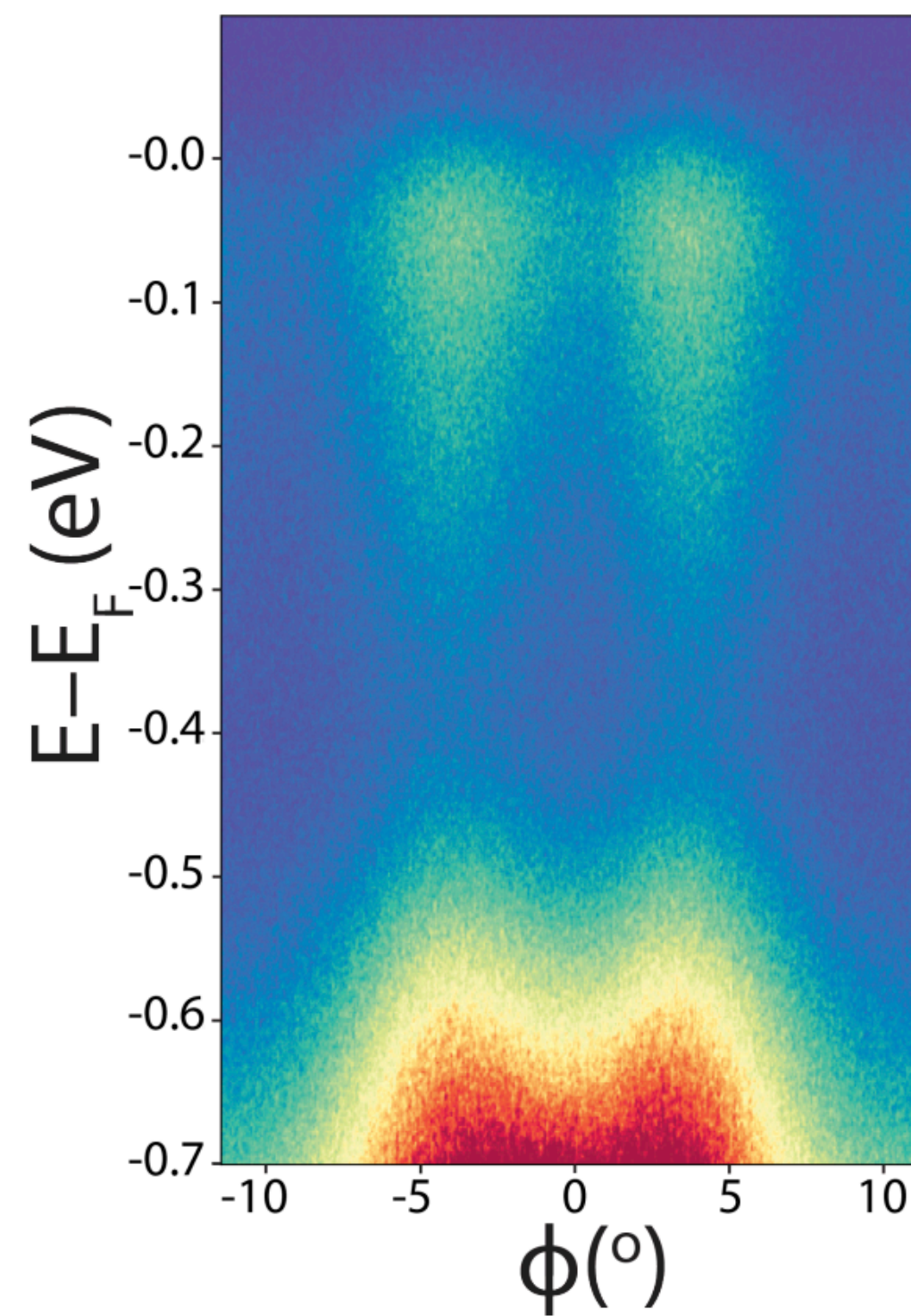
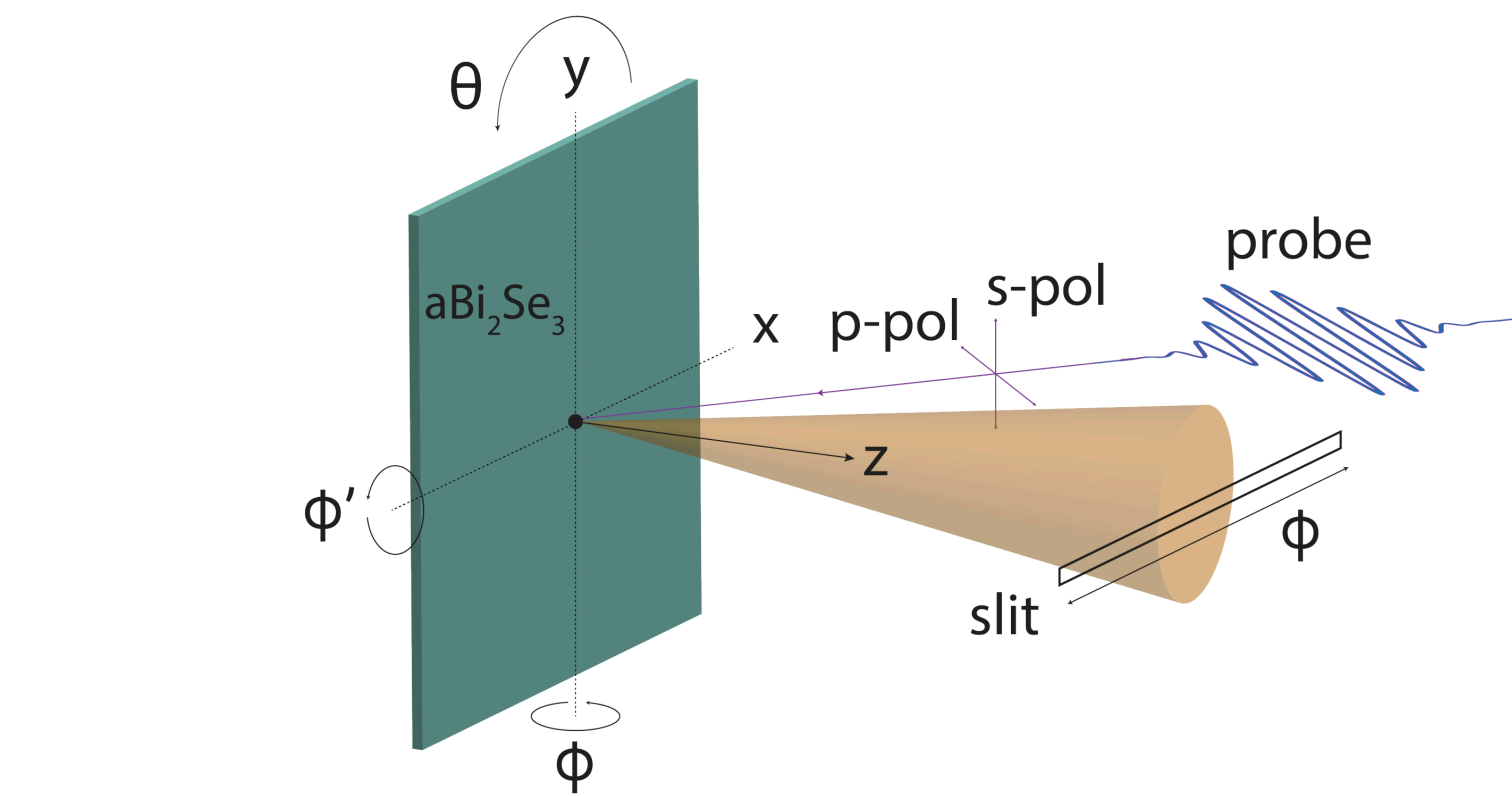
## Transport



Weak anti-localization at low T

Two decoupled channel conduction

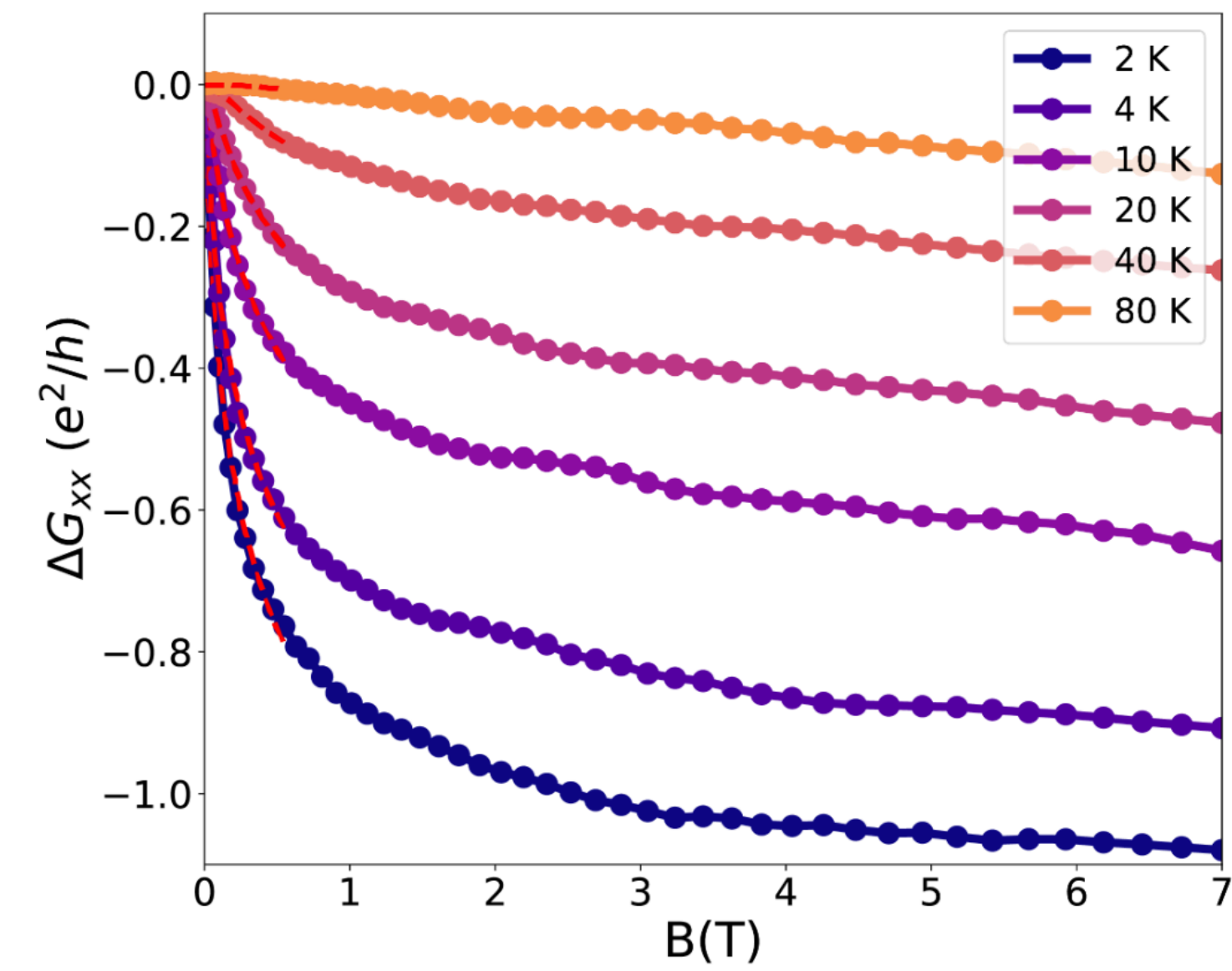
## ARPES



## spin resolved ARPES

# Amorphous $\text{Bi}_2\text{Se}_3$

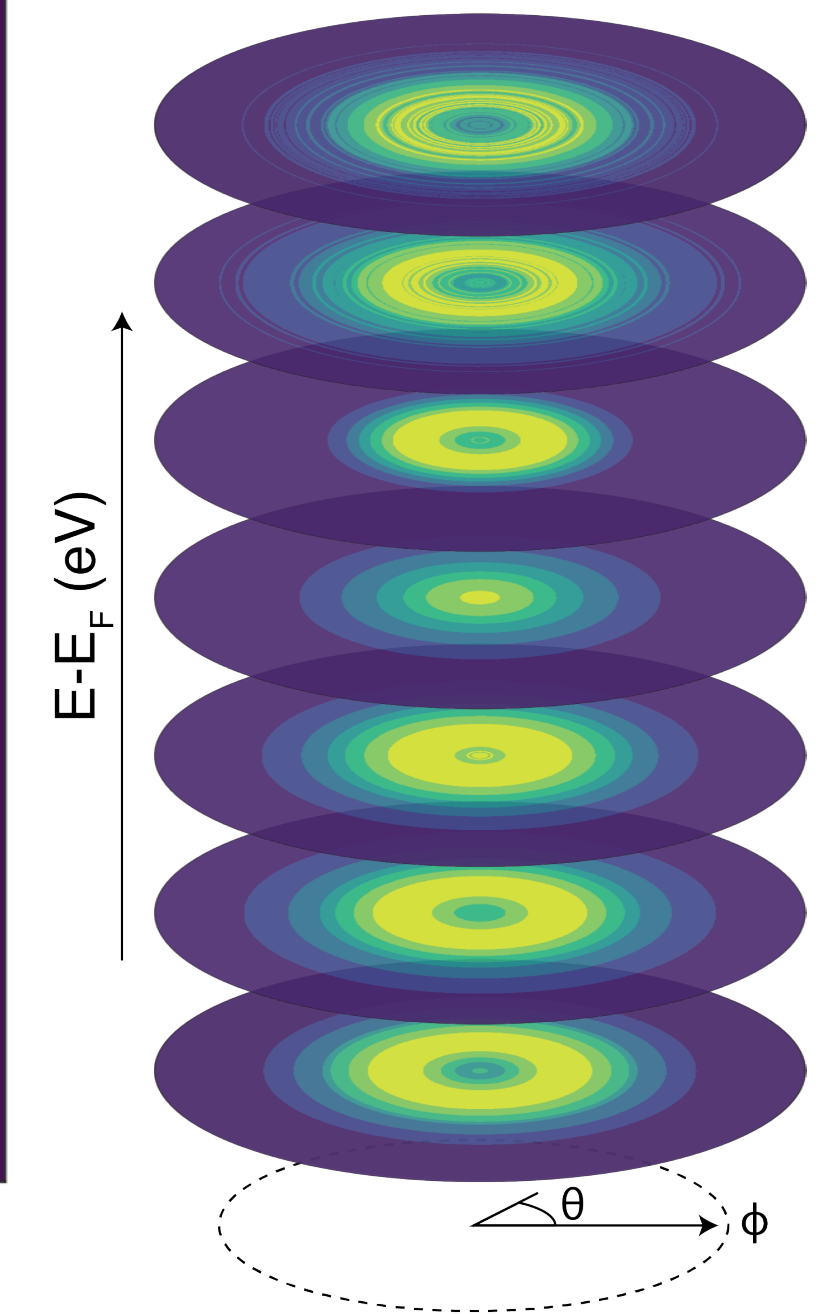
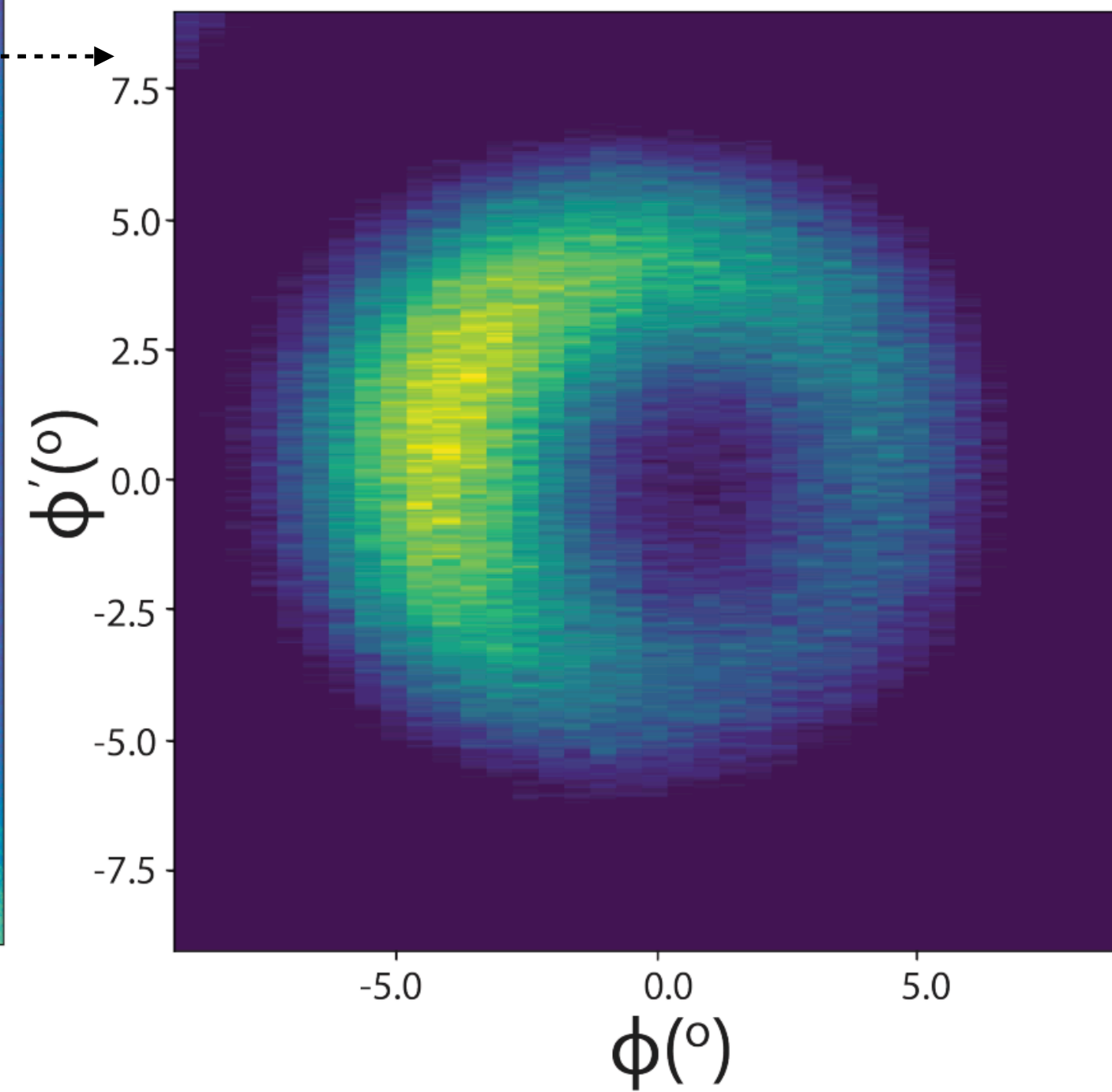
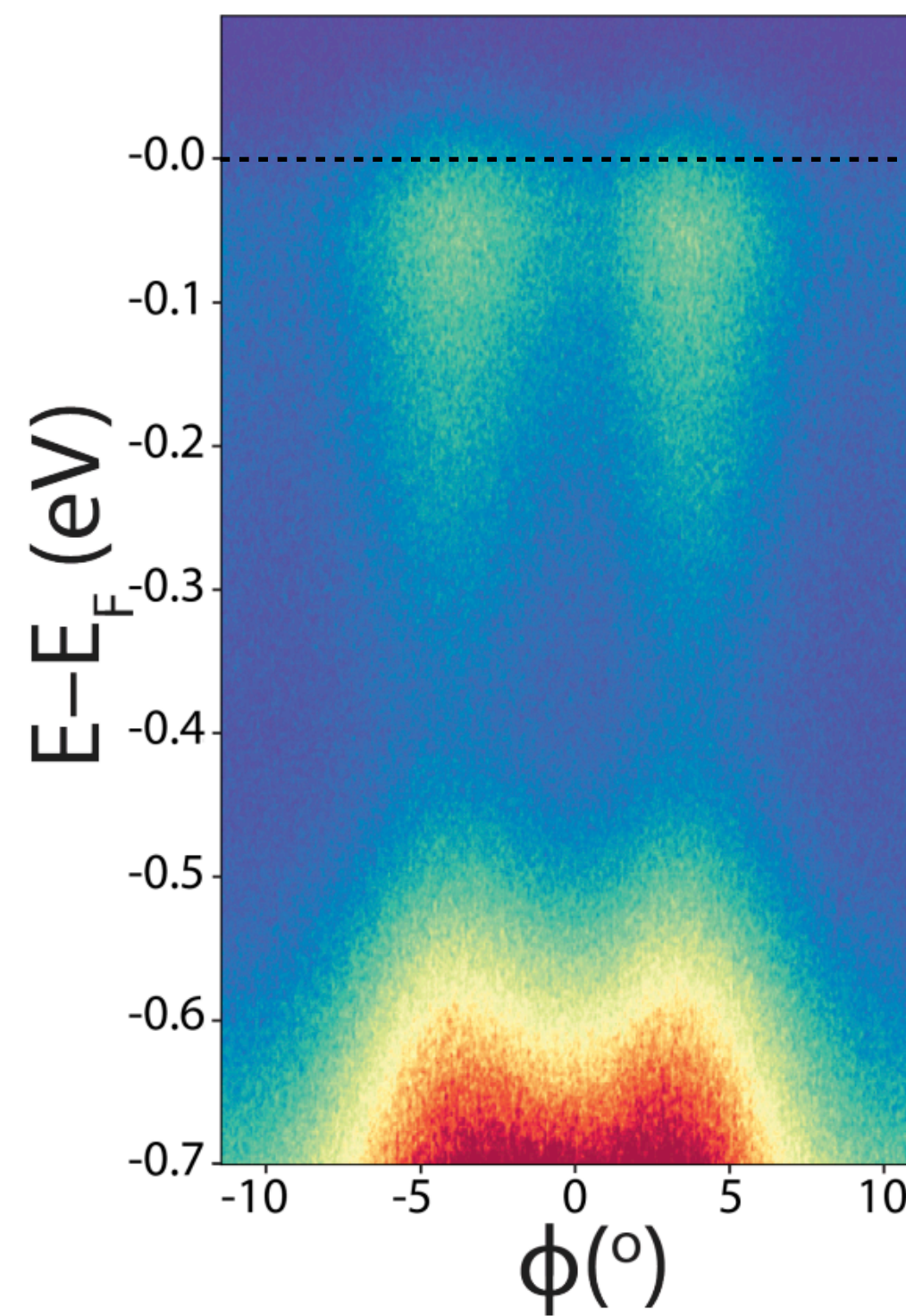
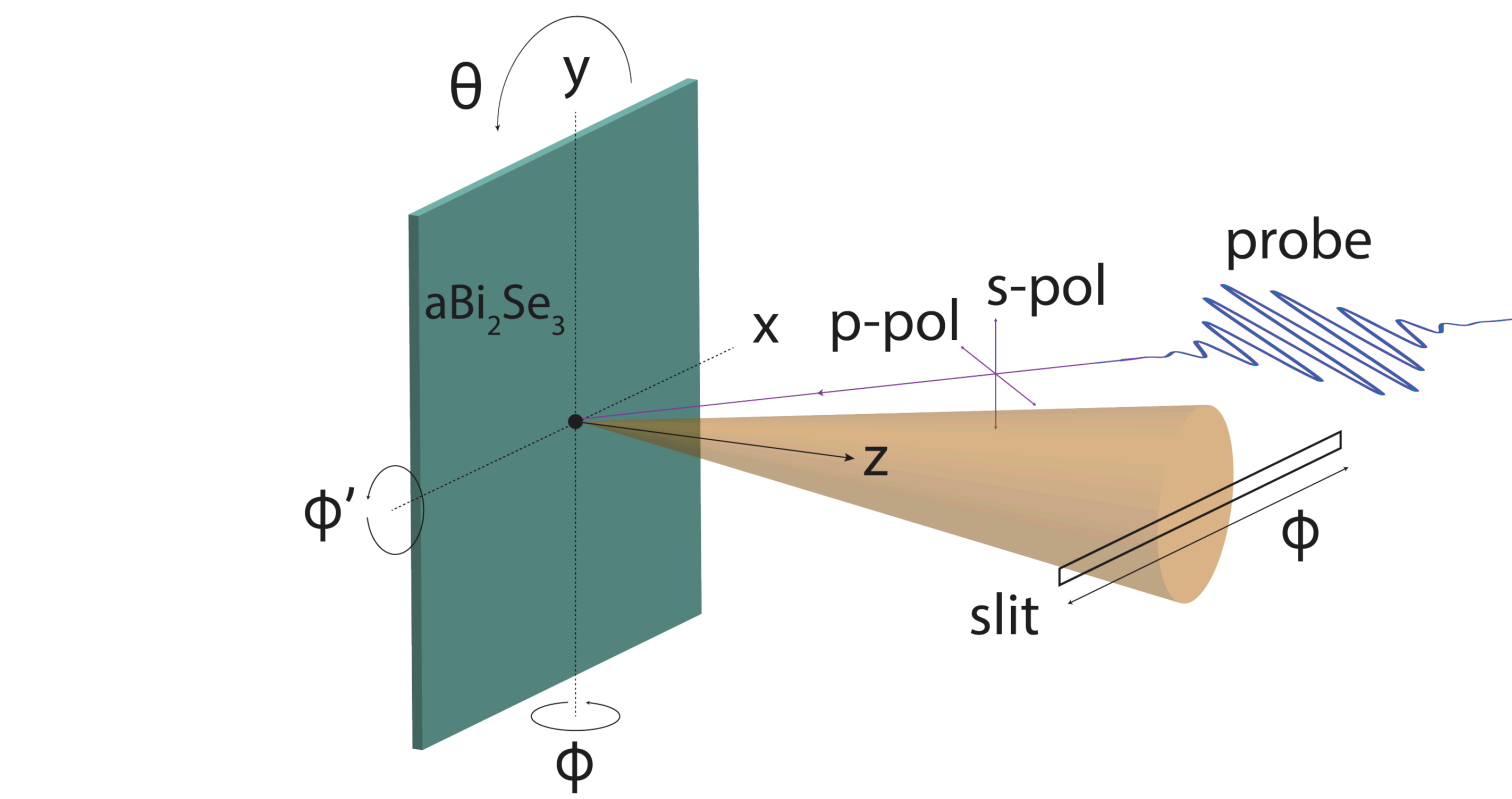
## Transport



Weak anti-localization at low T

Two decoupled channel conduction

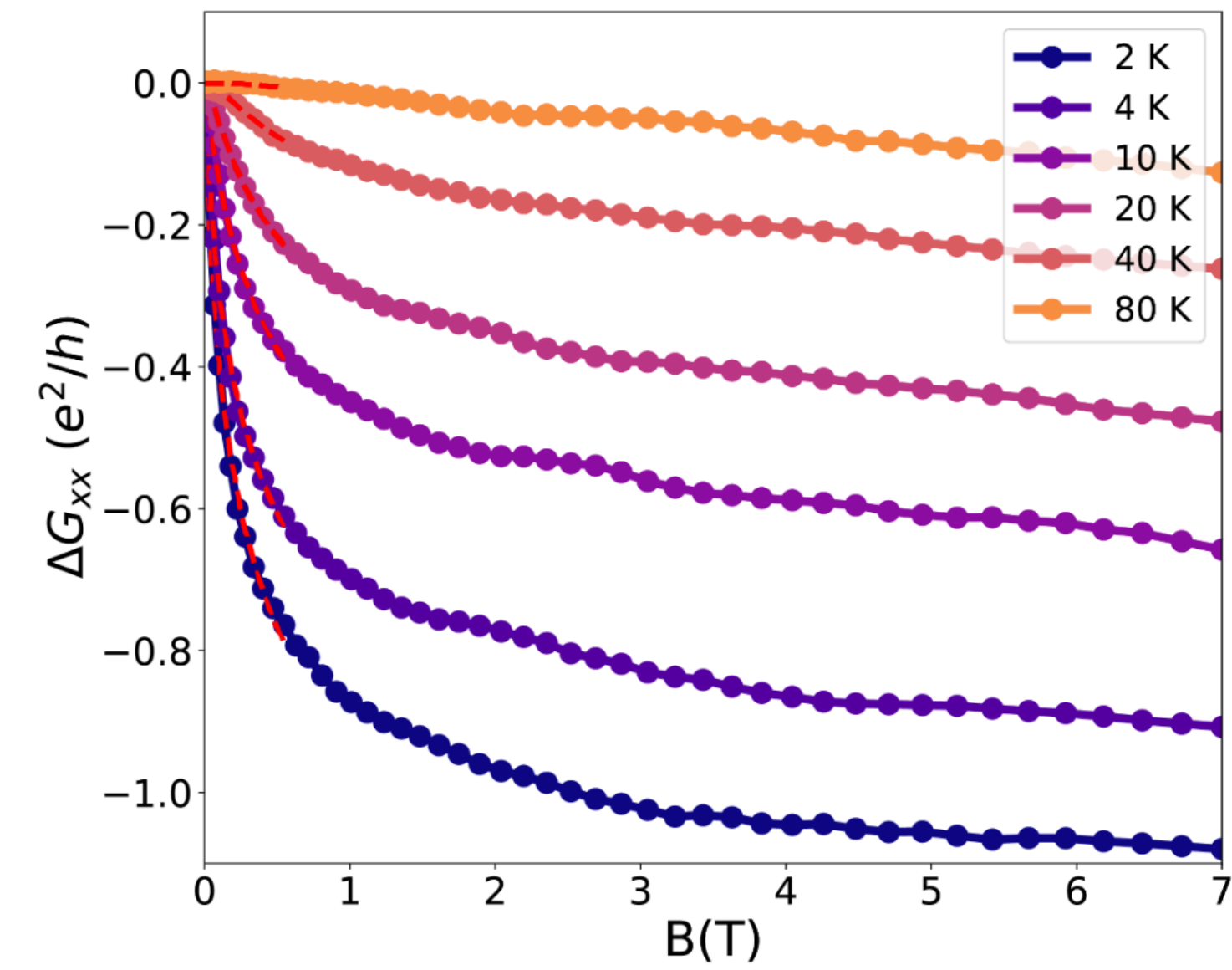
## ARPES



## spin resolved ARPES

# Amorphous $\text{Bi}_2\text{Se}_3$

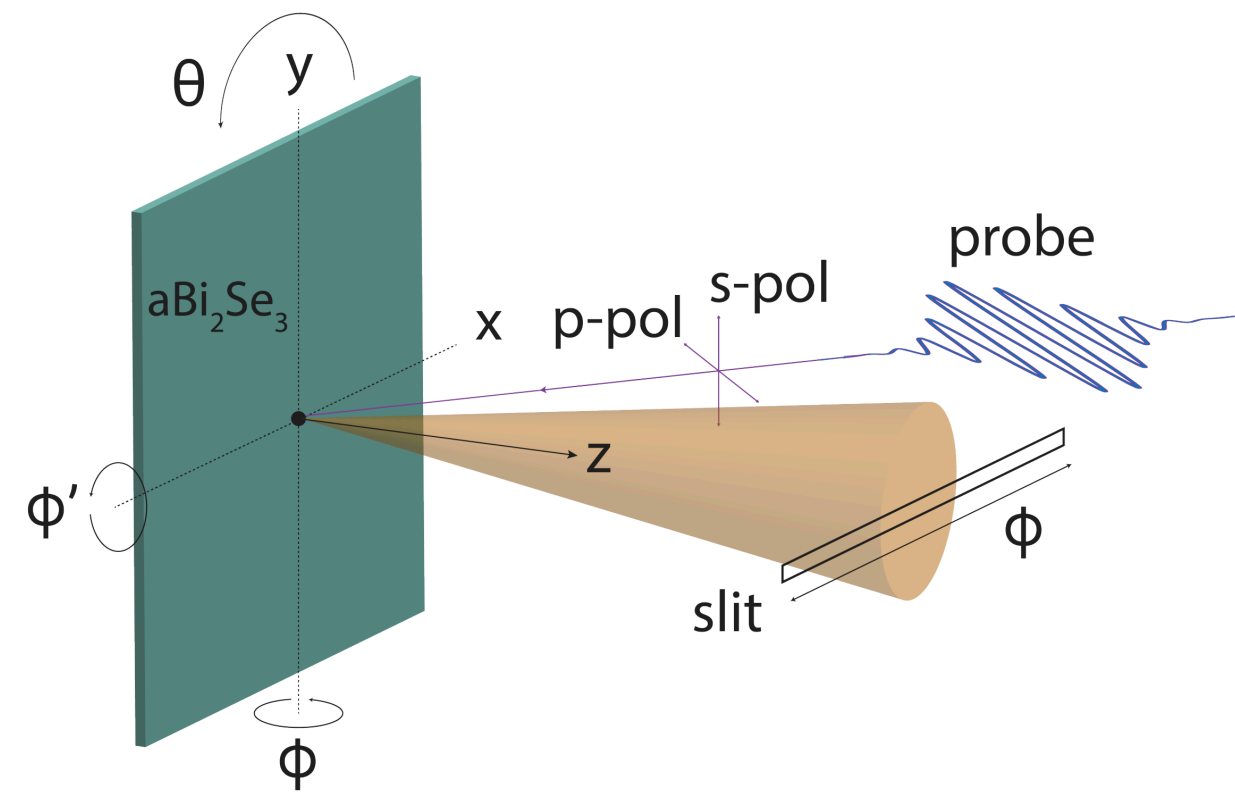
## Transport



Weak anti-localization at low T

Two decoupled channel conduction

## ARPES



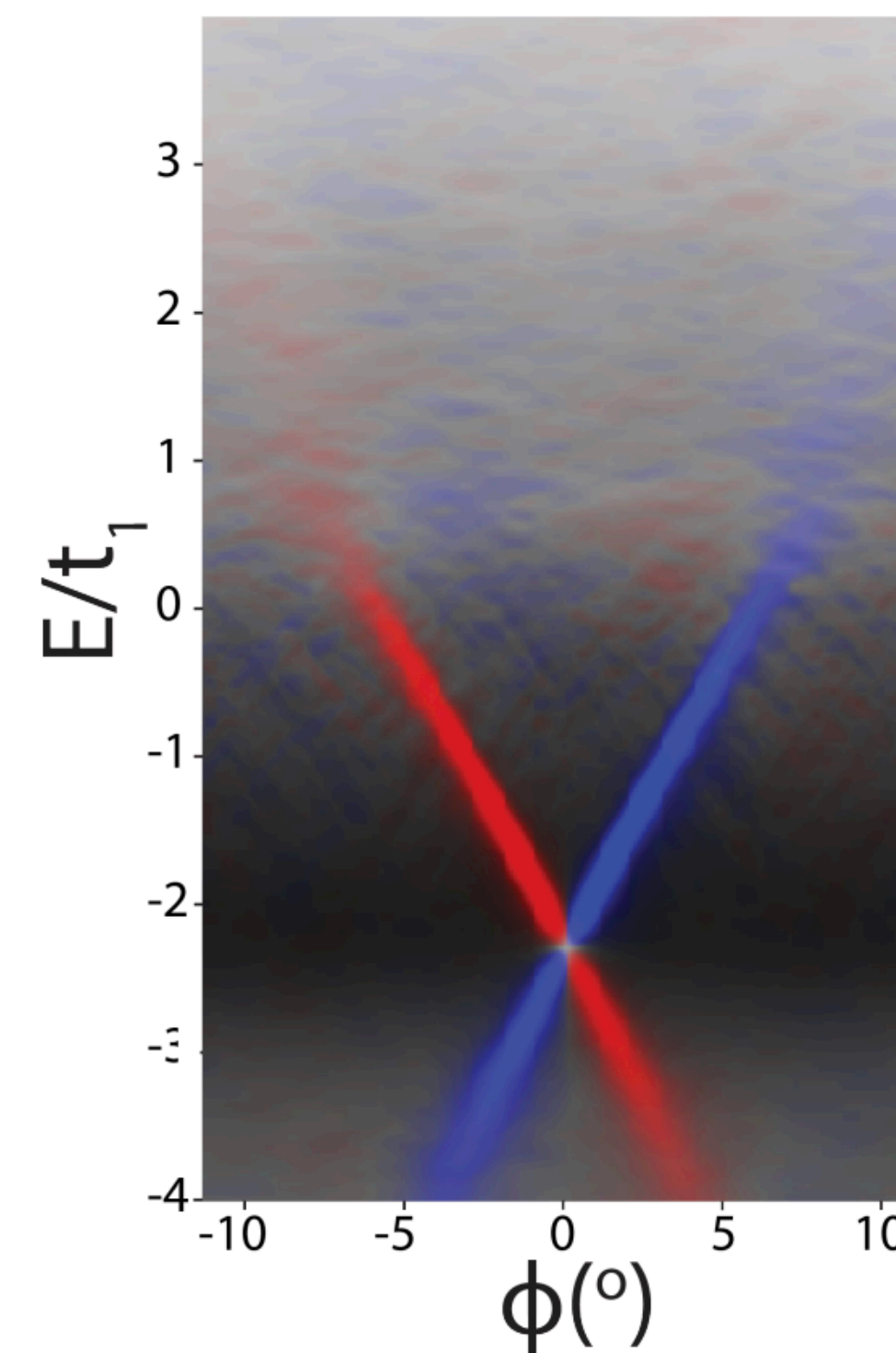
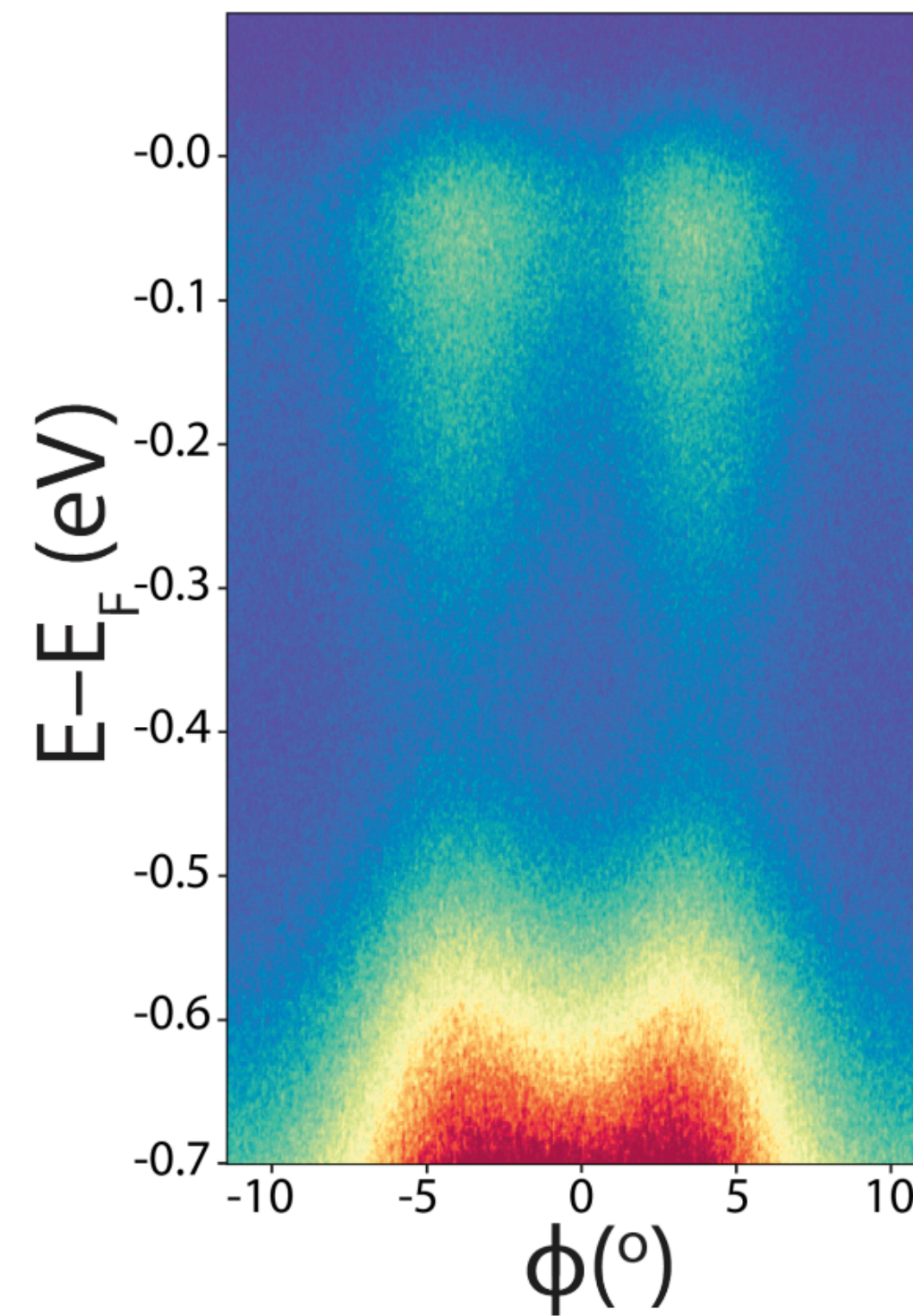
## spin resolved ARPES

### Theory

6-coordinated amorphous BHZ

Spectral function obtained by projecting to a plane-wave basis

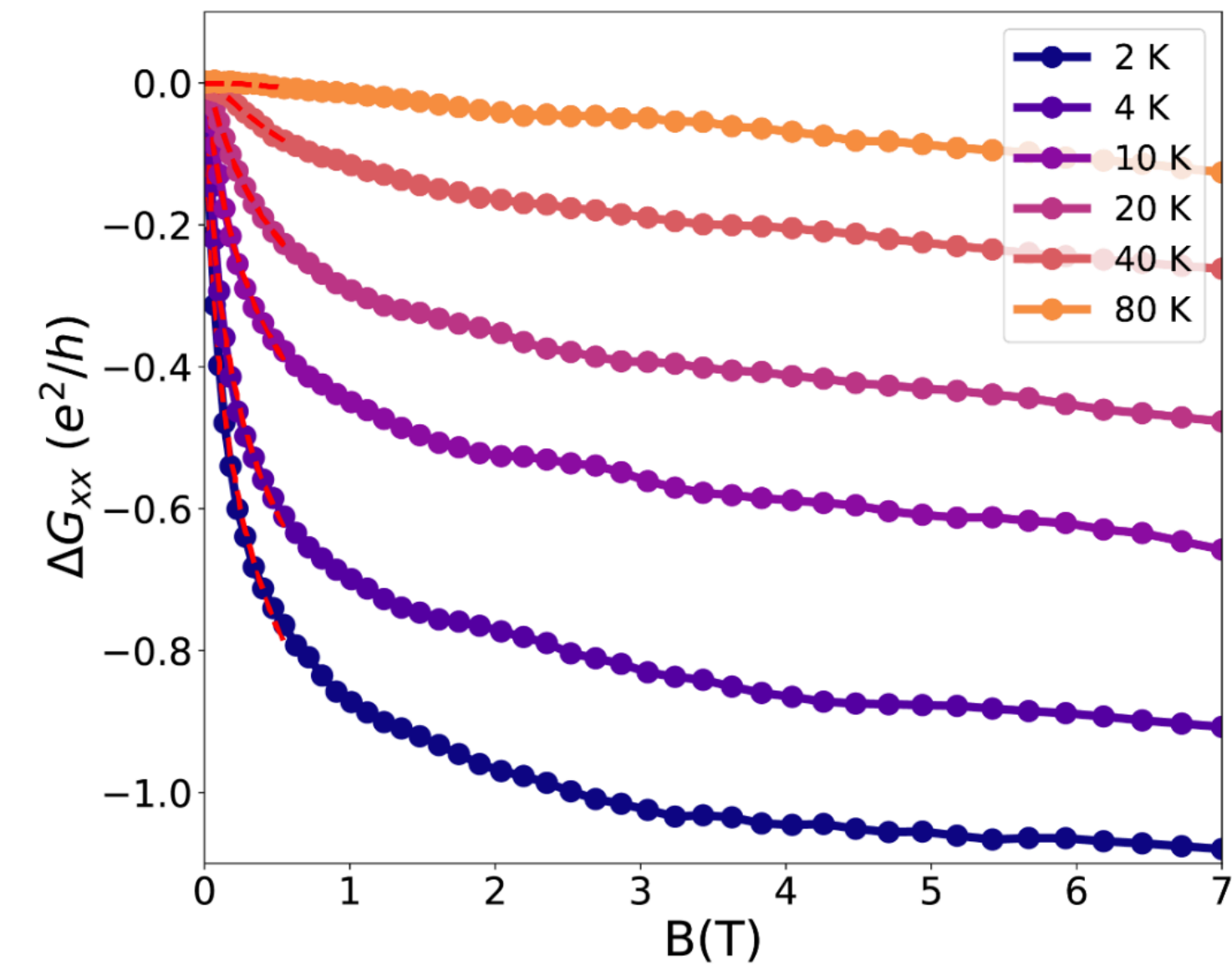
$$A(\mathbf{k}, E) = \sum_l \langle \mathbf{k}, l | \delta(H - E) | \mathbf{k}, l \rangle$$





# Amorphous $\text{Bi}_2\text{Se}_3$

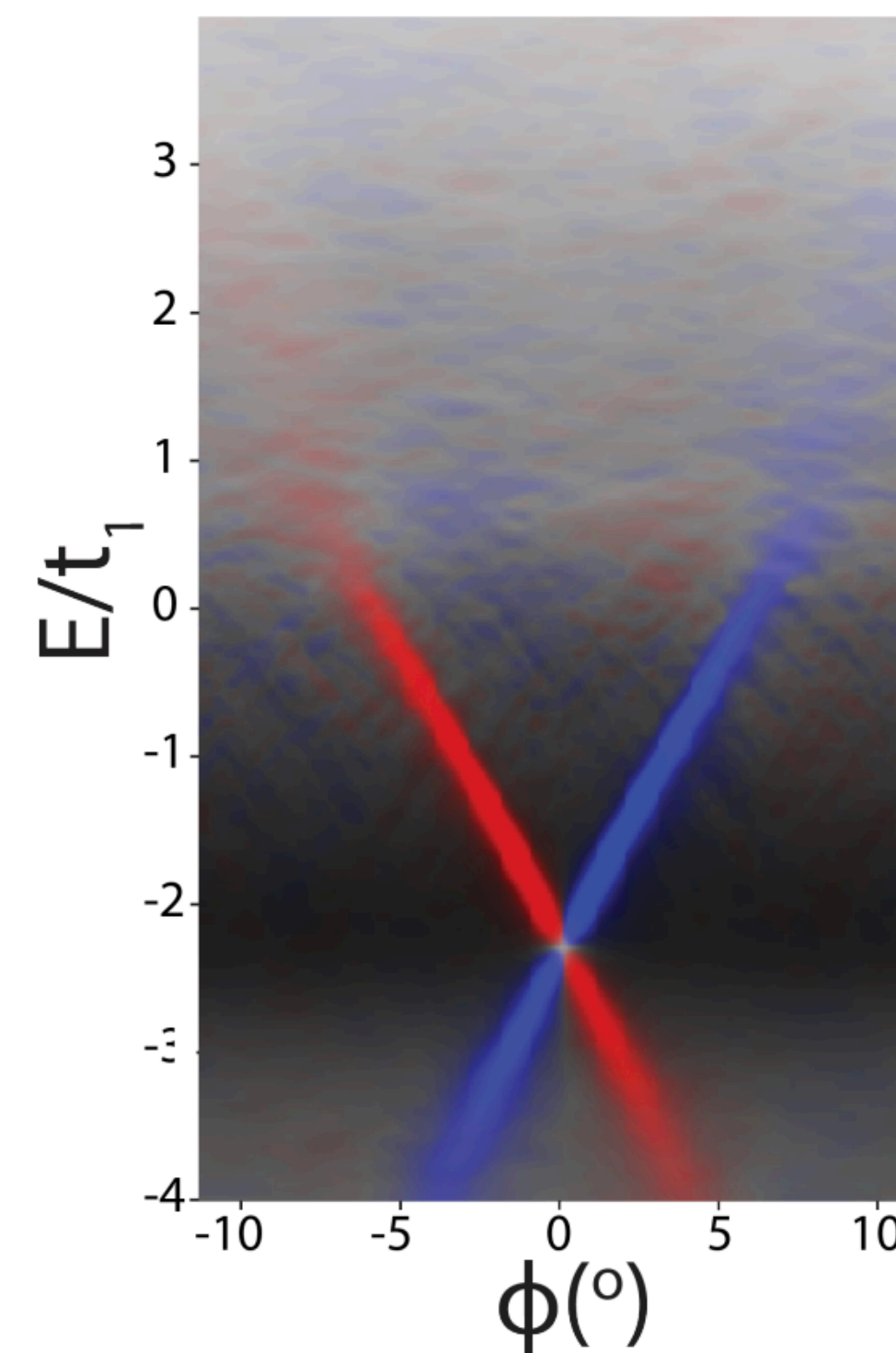
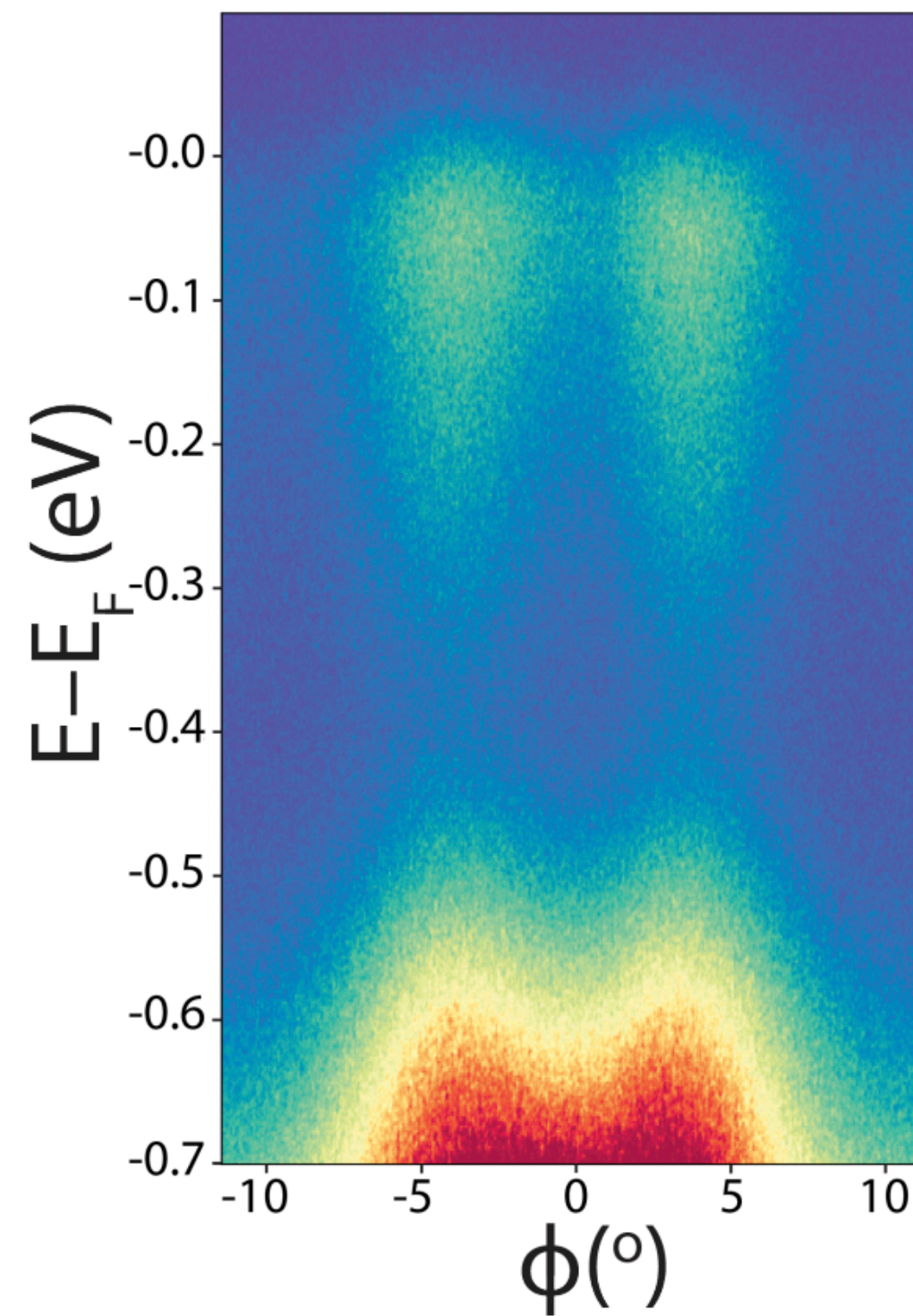
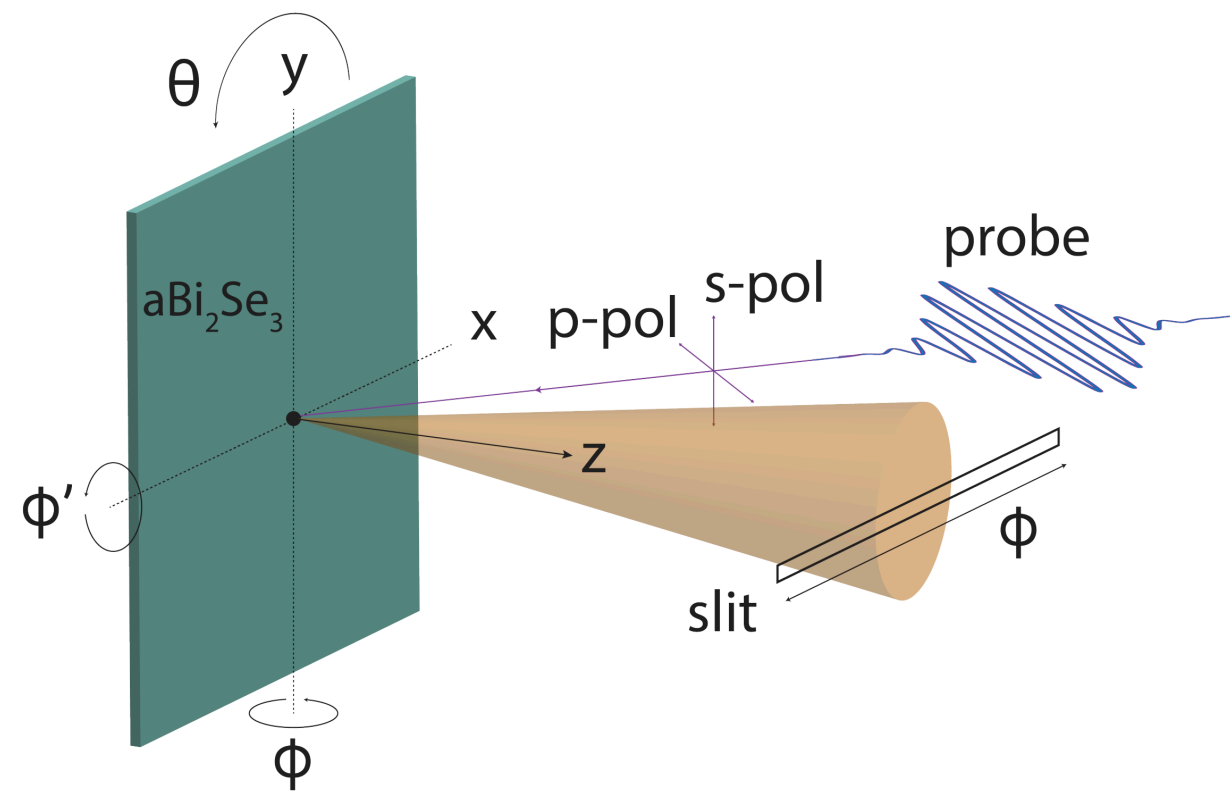
## Transport



Weak anti-localization at low T

Two decoupled channel conduction

## ARPES



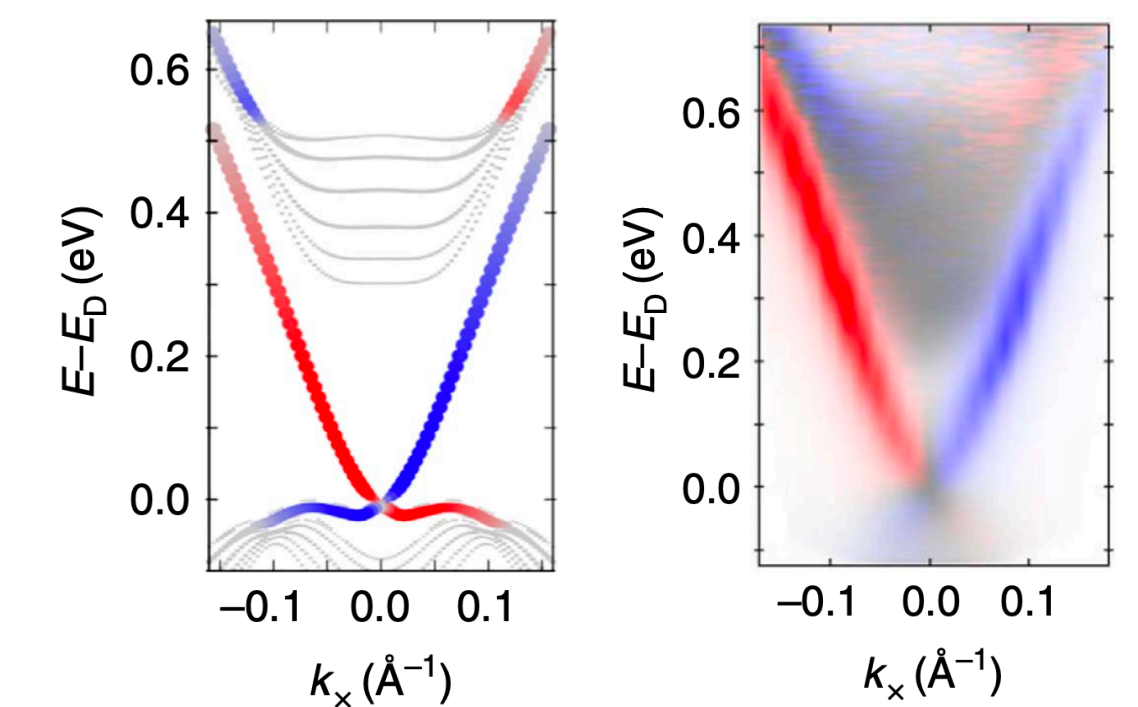
## Theory

6-coordinated amorphous BHZ

Spectral function obtained by projecting to a plane-wave basis

$$A(\mathbf{k}, E) = \sum_l \langle \mathbf{k}, l | \delta(H - E) | \mathbf{k}, l \rangle$$

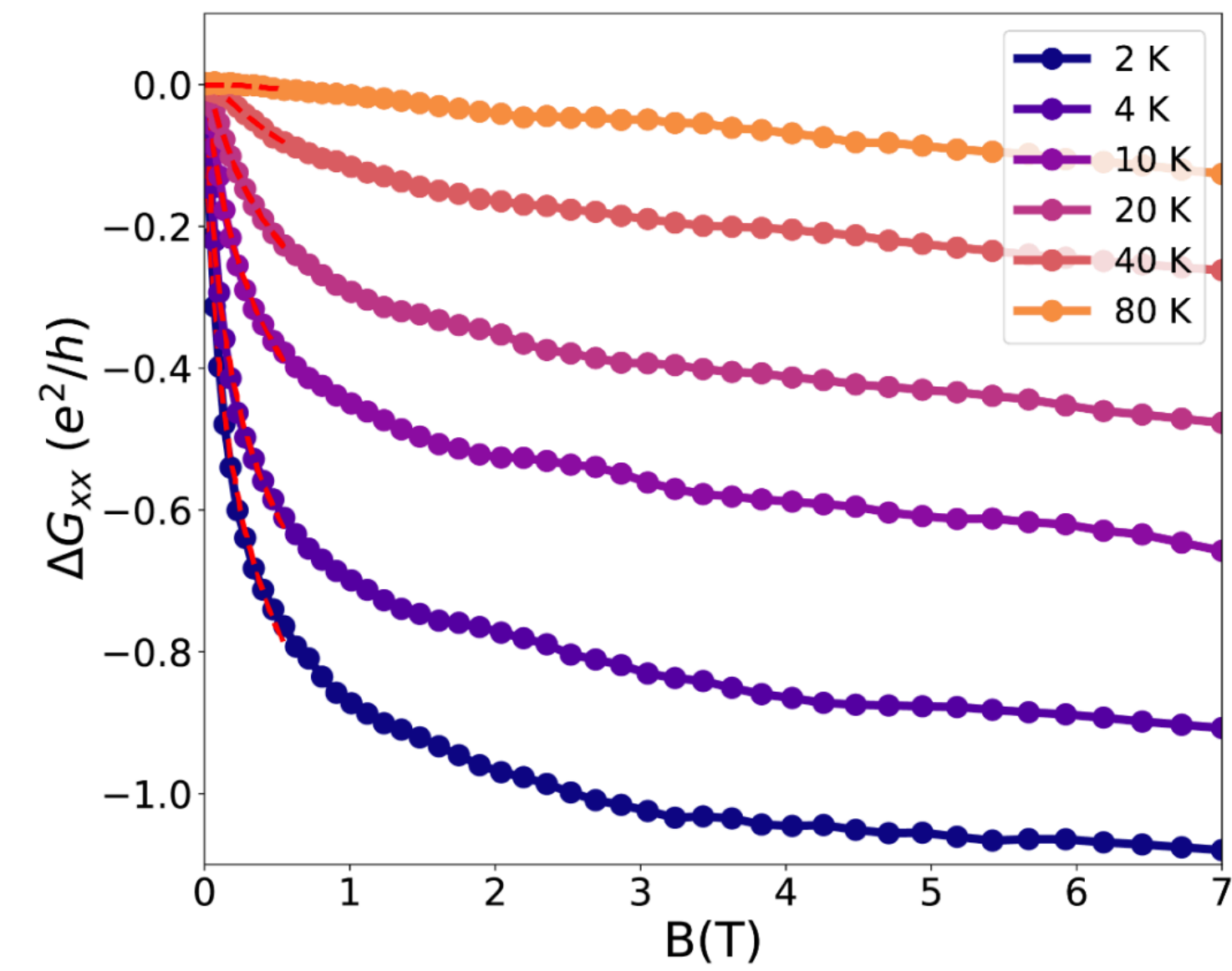
~ Crystal  $\text{Bi}_2\text{Se}_3$



Jozwiak, C. et al. Nat. Comm (2016)

# Amorphous $\text{Bi}_2\text{Se}_3$

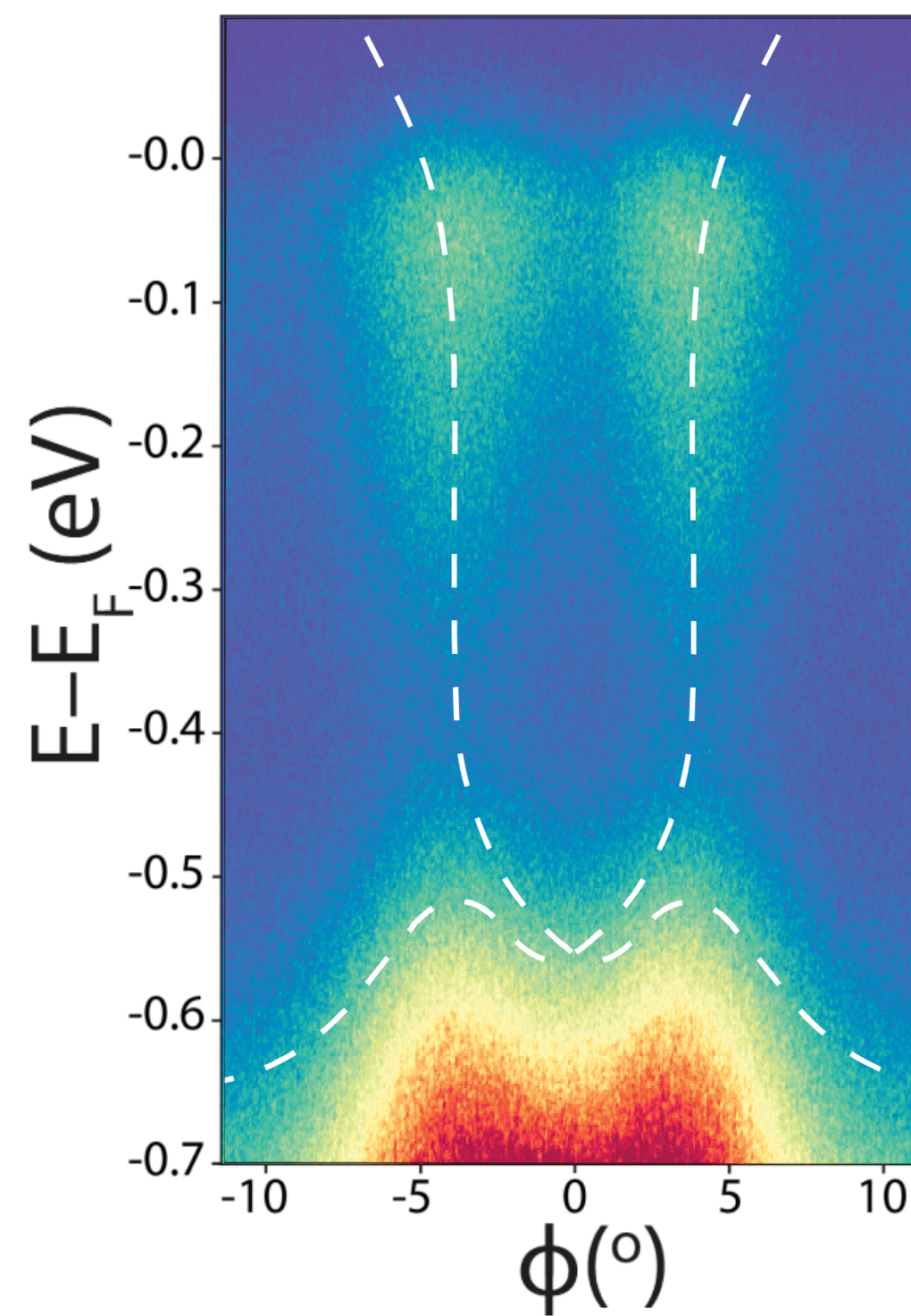
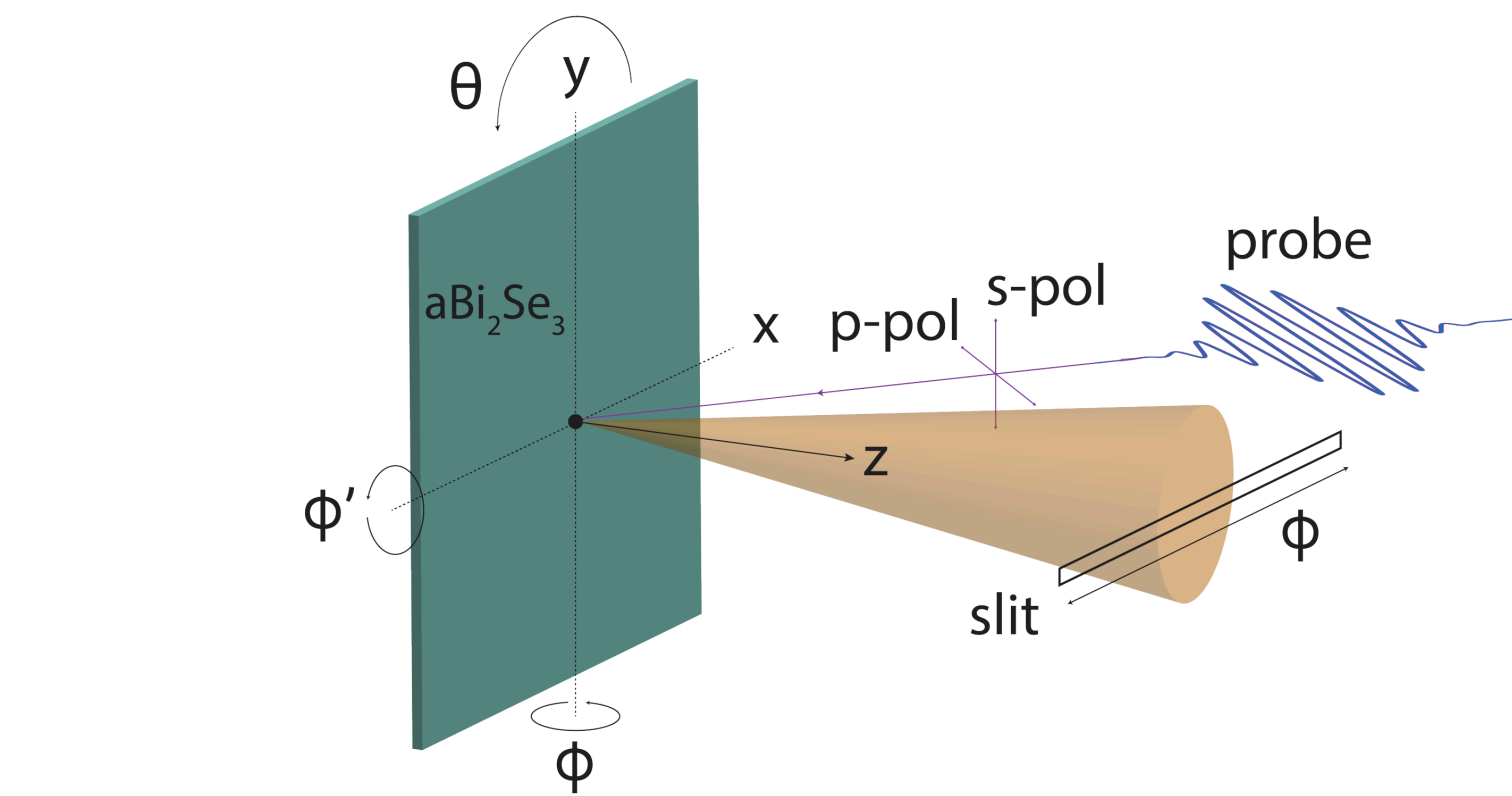
## Transport



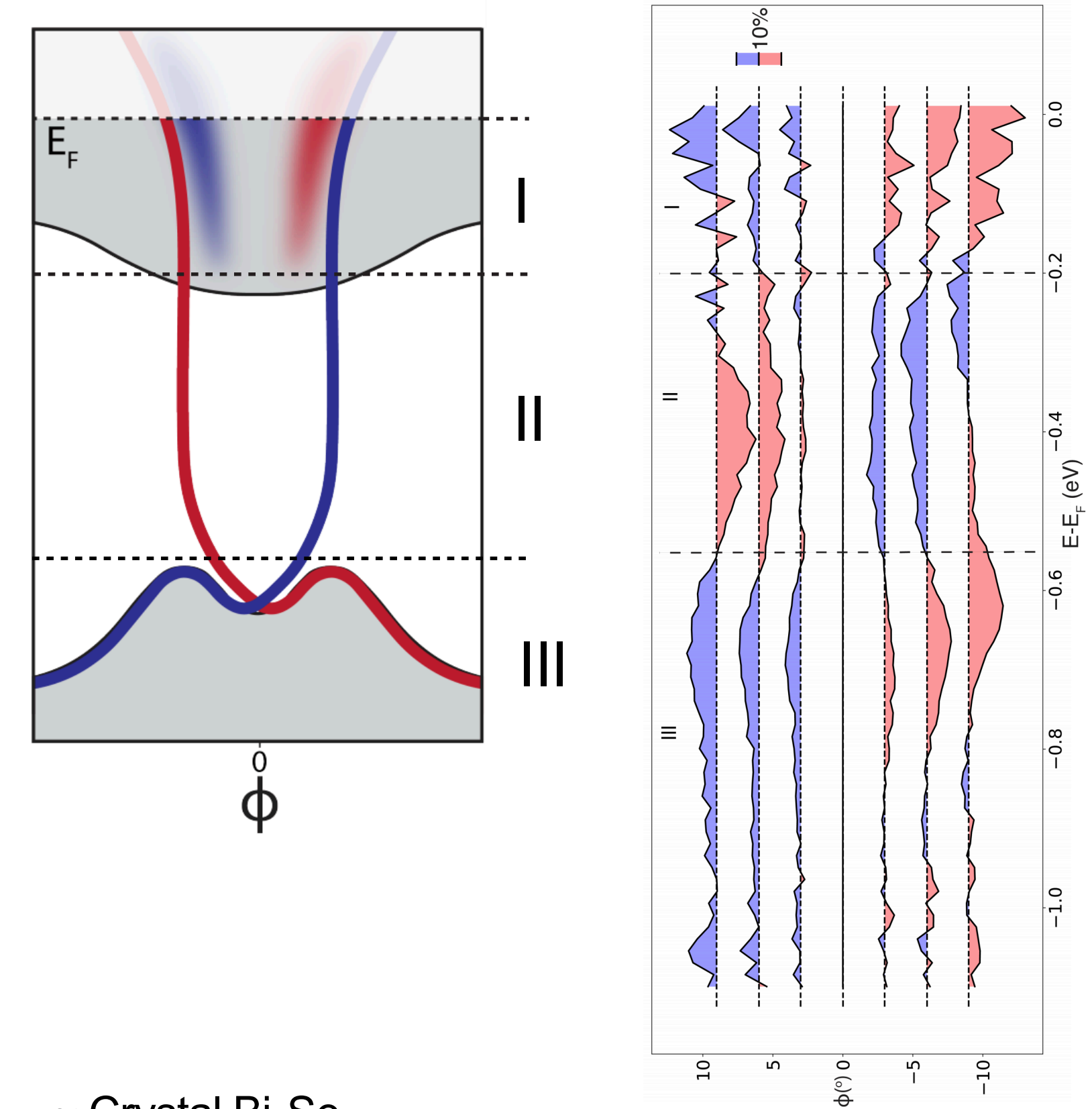
Weak anti-localization at low T

Two decoupled channel conduction

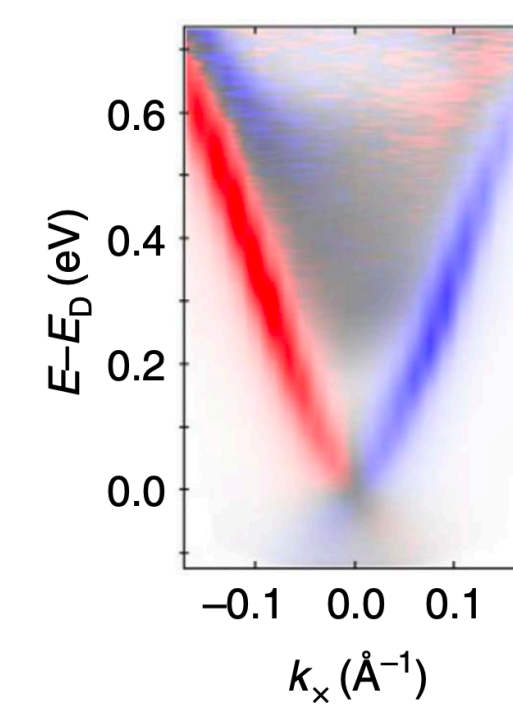
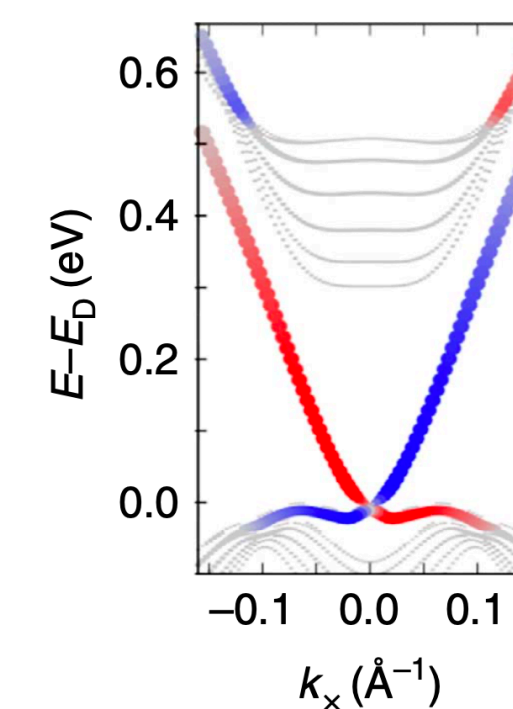
## ARPES



## spin resolved ARPES

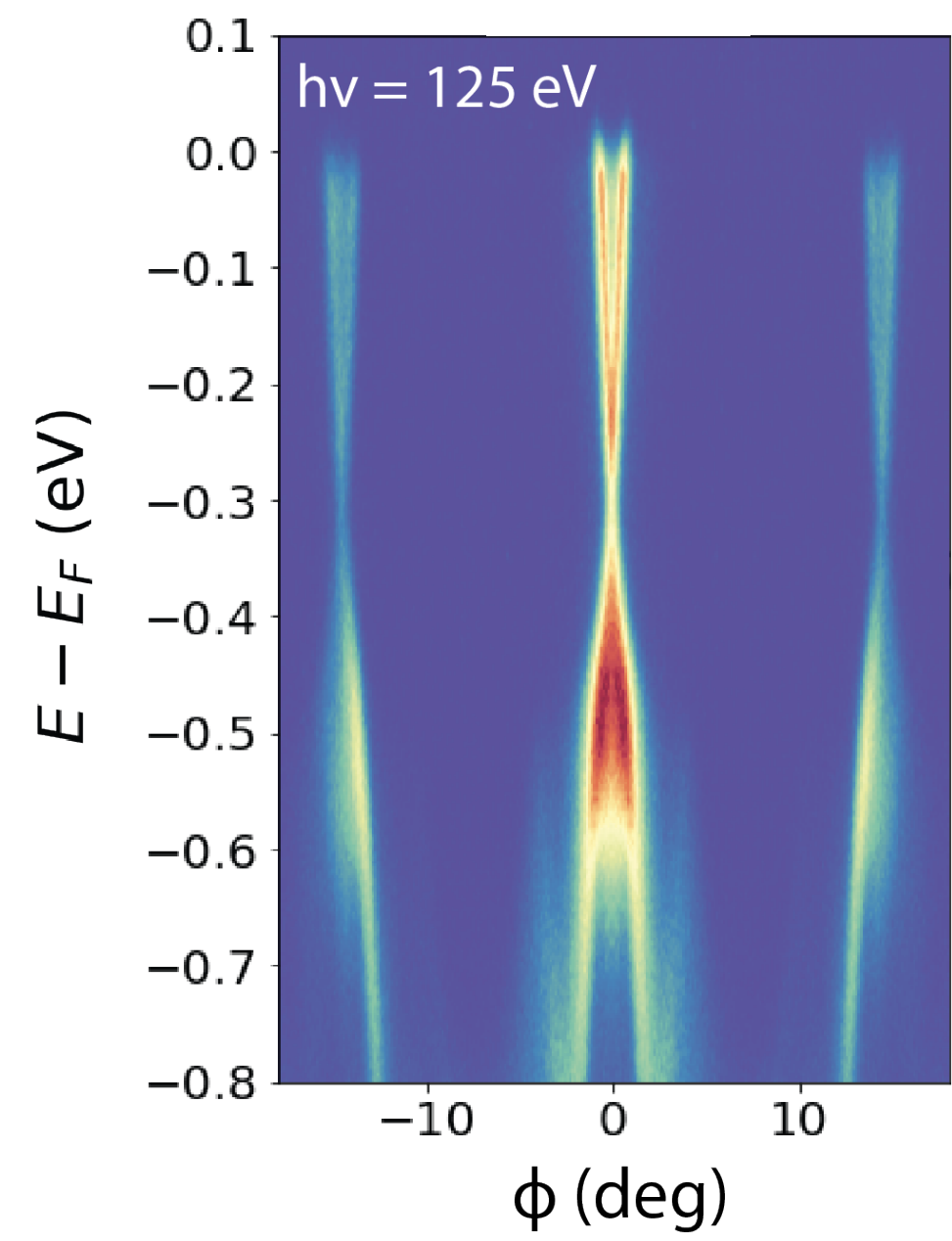
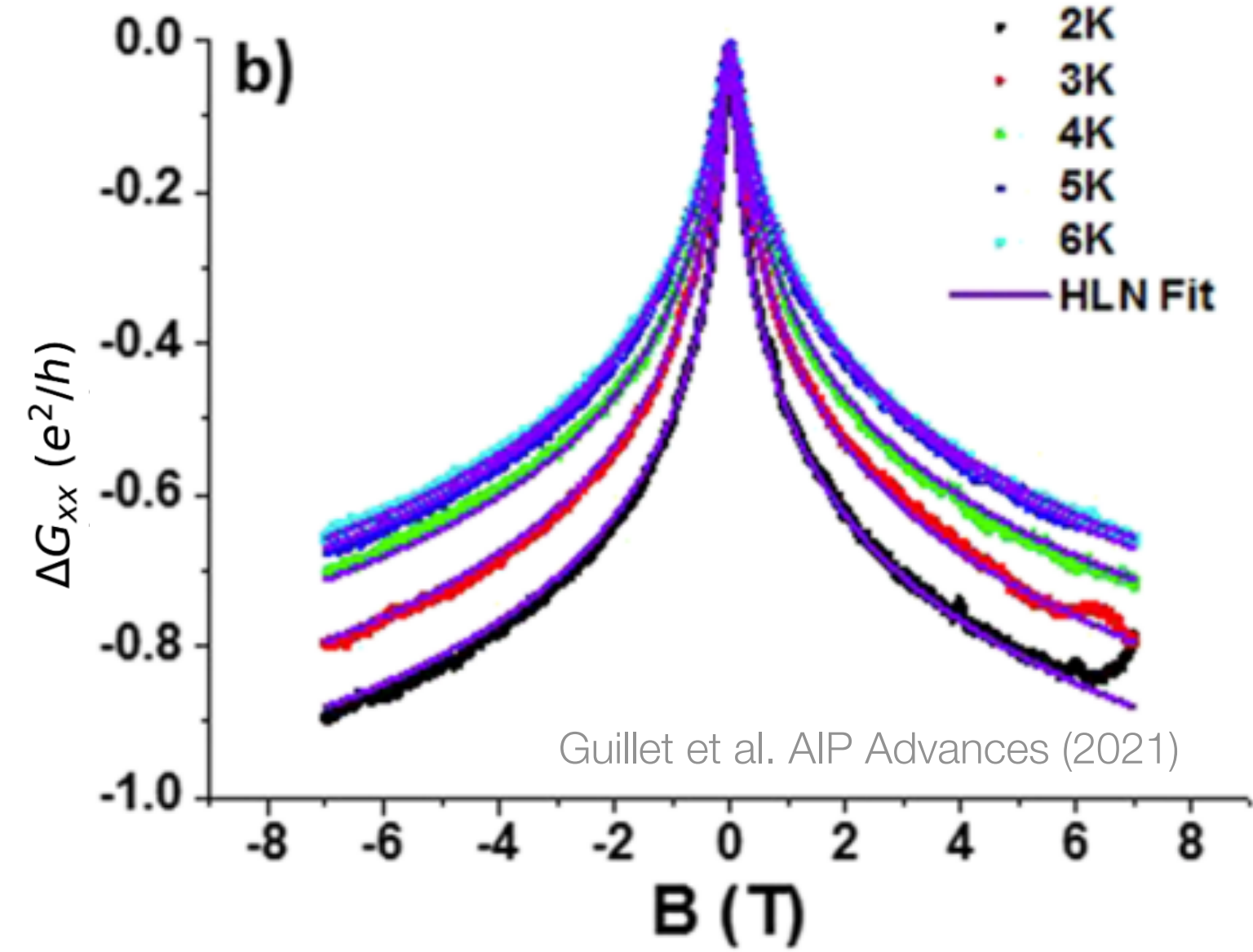


~ Crystal  $\text{Bi}_2\text{Se}_3$

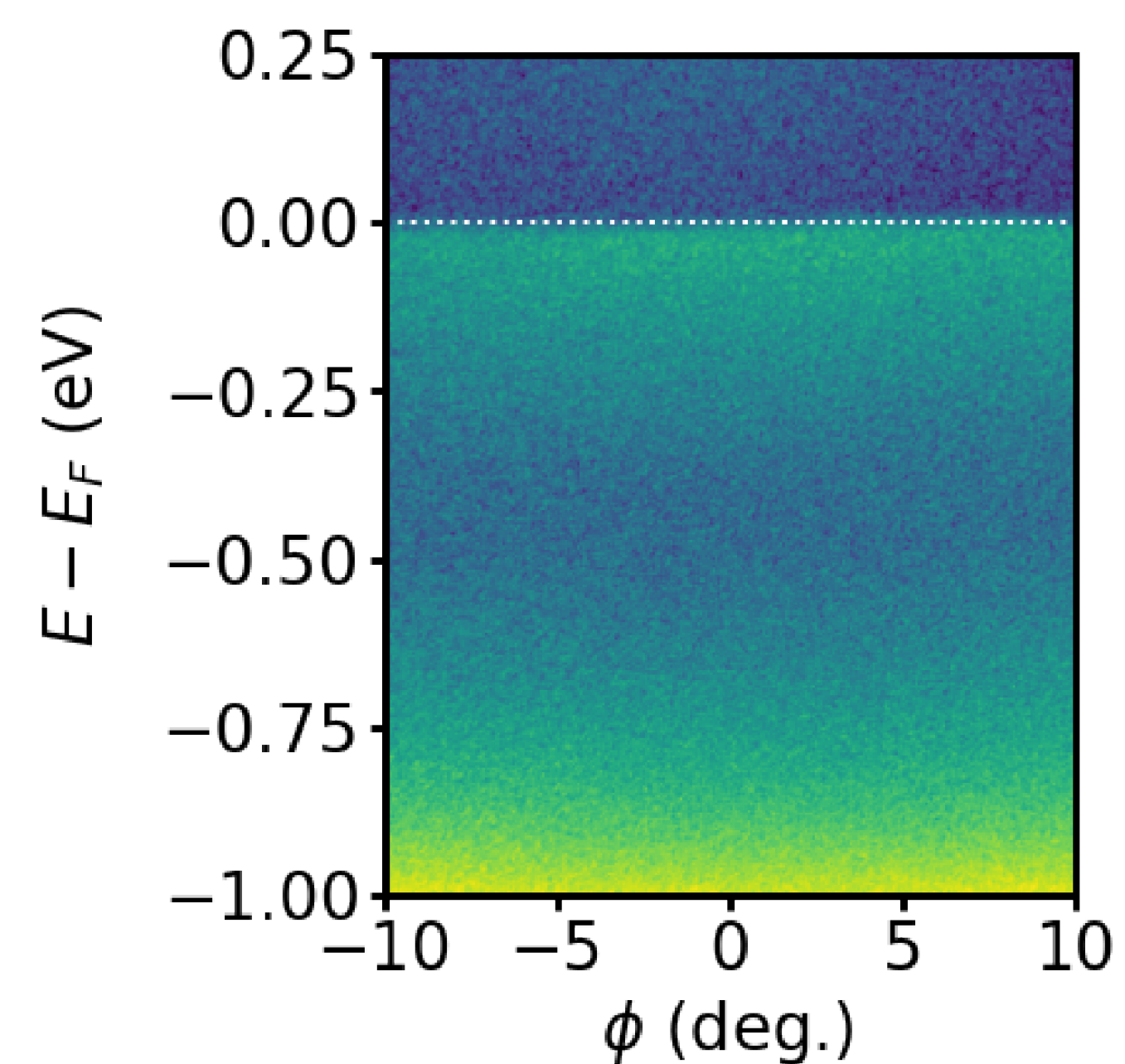
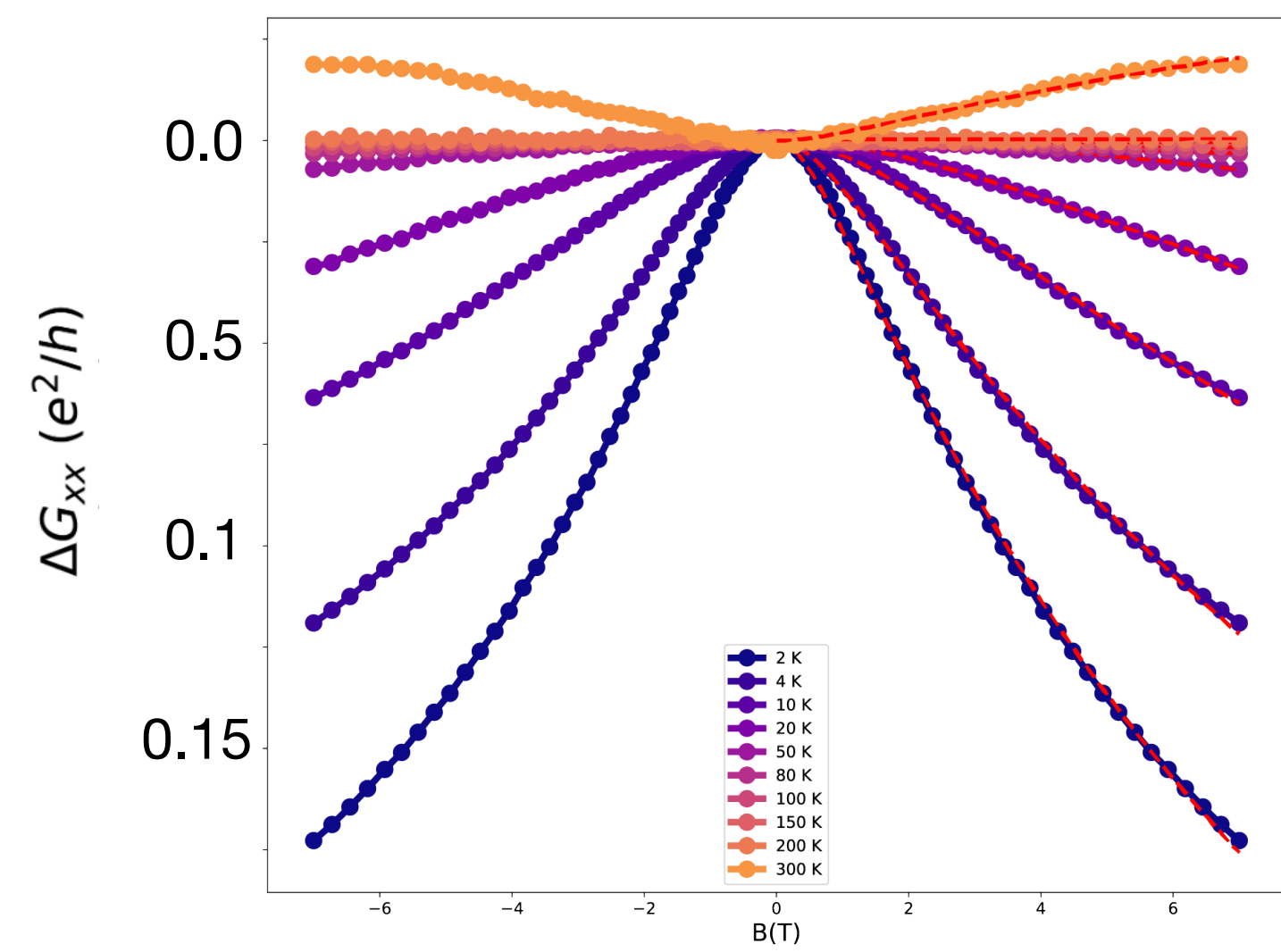


Jozwiak, C. et al. Nat. Comm (2016)

# Crystalline



# Polycrystalline



# Amorphous

