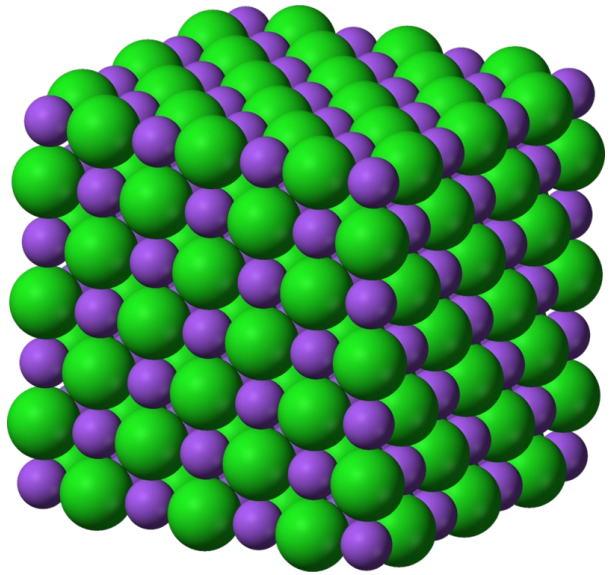
Topological phases of crystalline materials



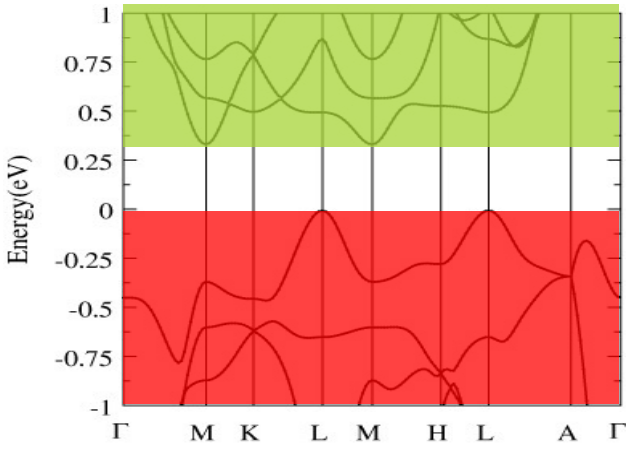
We know bulk invariants for perfect crystals

- Berry Curvature (Chern number, winding numbers, etc.)
- Symmetry Indicators

Band structure description

Enough to know one unit cell

Computationally cheap



Conduction band

Gap

Valence band

Ryu *et al.* New Journal of Physics, 12:065010 (2010)
A. Kitaev. AIP Conf. Proc., 1134:22–30 (2009)

	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

Topological phases beyond perfect crystals

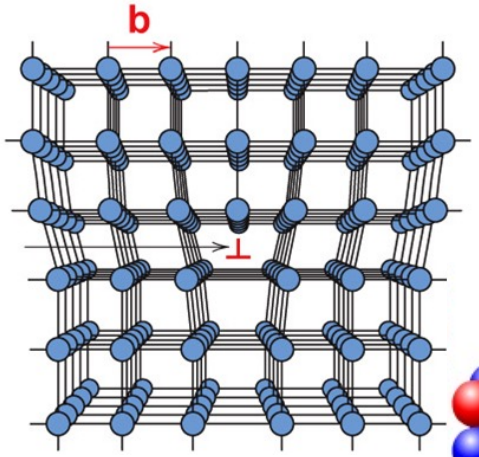
Lattice defects

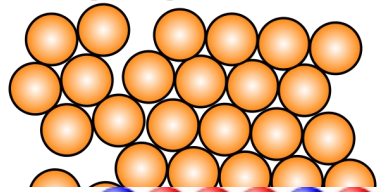
Amorphous materials

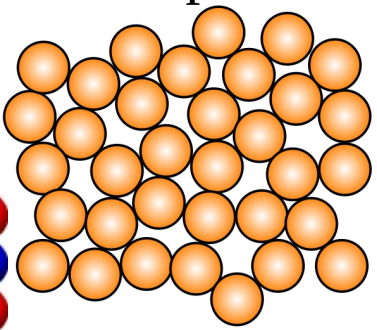
Many known TI's are alloys:

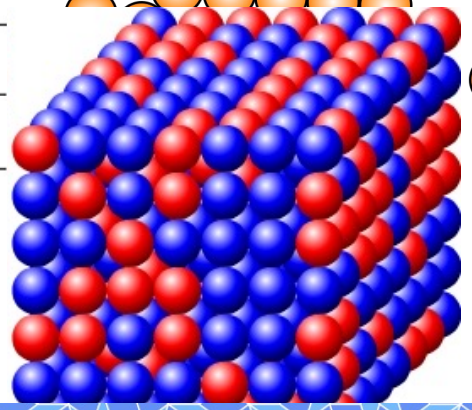
Bi_xSb_{1-x}, $Sn_xPb_{1-x}Te$

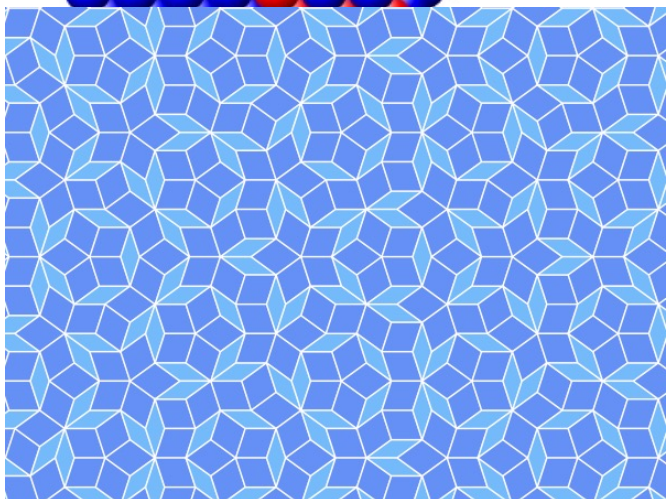
Quasicrystals











Need new methods to discover aperiodic topological materials:

- Local topological markers
- Effective Hamiltonian symmetry indicators

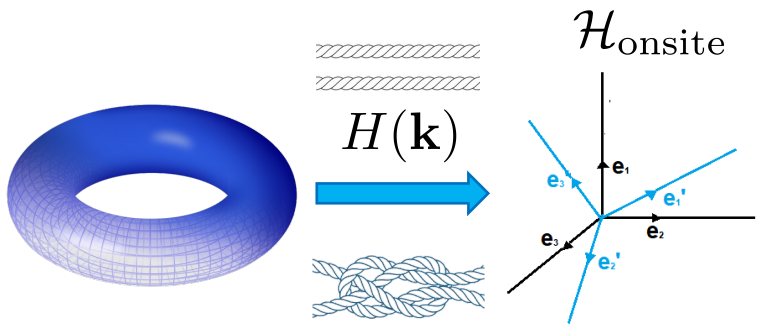
- Numerics: Kernel Polynomial Method

Real-space topological invariants in disordered systems

Crystals: Chern number [TKNN PRL **49** 405 (1982)]

$$\sigma_{xy} = \frac{dj_x}{dE_y} = \frac{e^2}{h} C$$

$$C = -\frac{1}{\pi} \mathrm{Im} \sum_{n \in \mathrm{occ.}} \int_{\mathrm{BZ}} \mathrm{d}\mathbf{k}^2 \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial k_x} \middle| \frac{\partial u_{n\mathbf{k}}}{\partial k_y} \right\rangle$$



Noncrystalline:

- Local Chern number/Chern marker
- Bott index
- Spectral localizer

Local Chern number/Chern marker

[Bianco, Resta PRB **84**, 241106 (2011)]

Projected position operators

$$\hat{X} = P\hat{x}P \qquad \hat{Y} = P\hat{y}P \qquad\qquad P = \sum_{n\in \mathrm{occ.}} |n\rangle\langle n|$$

Local Chern number defined deep in the bulk:

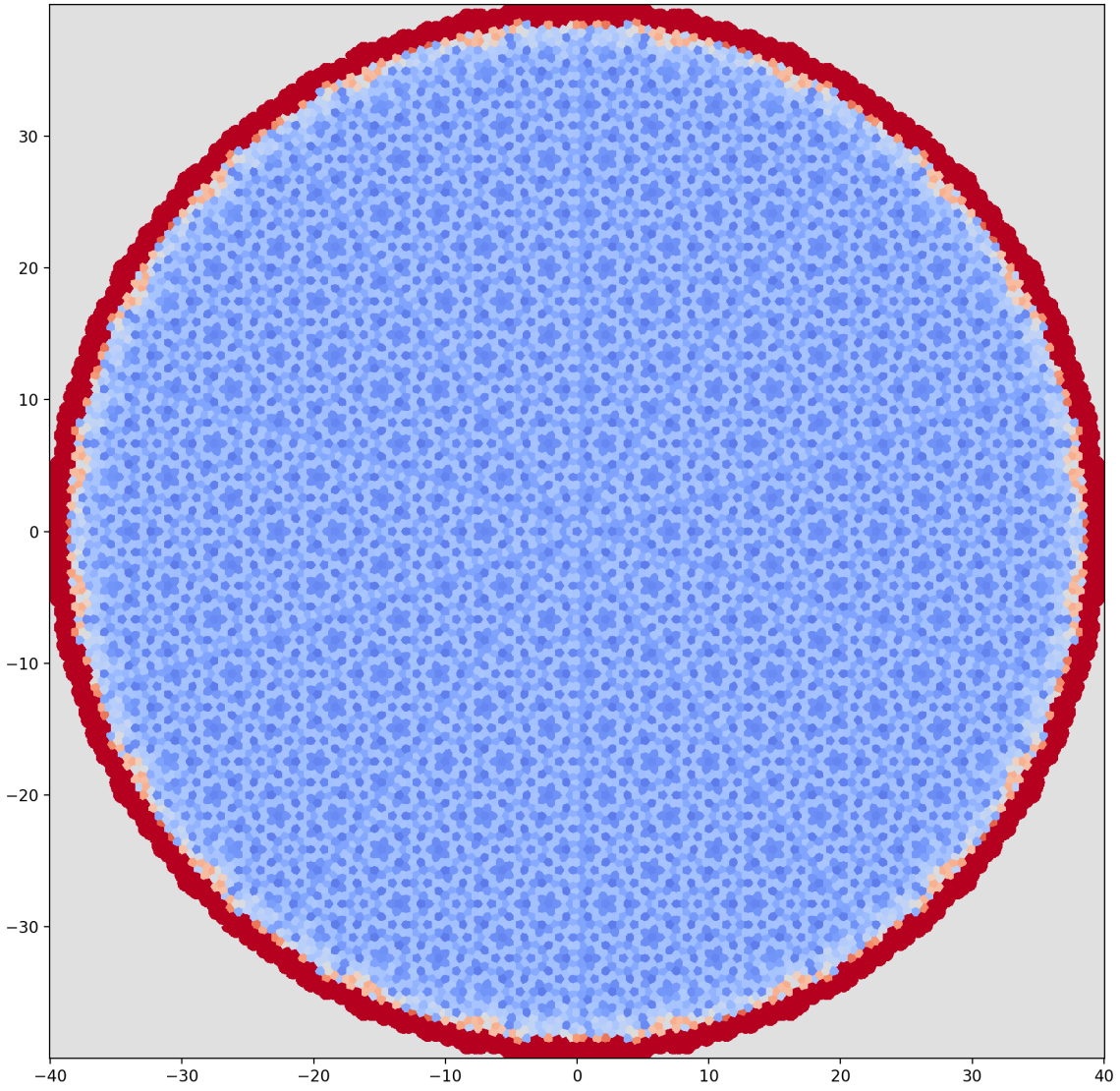
$$C(\mathbf{r}) = -\frac{2\pi i}{A_{\mathrm{cell}}} \langle \mathbf{r}| \left[\hat{X}, \hat{Y}\right] |\mathbf{r}\rangle$$

Local Hall conductivity

$$\sigma_{xy}(\mathbf{r}) = \frac{dj_x(\mathbf{r})}{dE_y} = \frac{e^2}{h} C(\mathbf{r})$$

Gives Chern number for crystalline system

Example: Local Chern number on quasicrystal using KPM



Integer quantum Hall state

Chern number in bulk averages to integer

$$C = -\frac{2\pi i}{A}\mathrm{Tr}_A\left(\left[\hat{X},\hat{Y}\right]\right)$$

KPM allows calculation in ξ^d time

(more on that later)

Quantized to 3 decimals

Generalization to other Z invariants

Bott index

[Loring, Hastings EPL 92 67004 (2010)]

Exponential projected position operators (with periodic boundary conditions)

$$\hat{U} = P \exp\left(\frac{2\pi i \hat{x}}{L_x}\right) P \qquad \hat{V} = P \exp\left(\frac{2\pi i \hat{y}}{L_y}\right) P \qquad P = \sum_{n \in \mathrm{occ.}} |n\rangle\langle n|$$

Global property of the periodic sample

$$\mathrm{Tr} \log\left(\hat{U}\hat{V}\hat{U}^{\dagger}\hat{V}^{\dagger}\right) = 2\pi i C + r$$

Generalizable to other symmetry classes

Spectral localizer

[Loring, Annals of Physics, Vol. 356, 383-416 (2015), Cerjan & Loring, arXiv:2411.03515 (2024)]

Define the combination of operators (with open boundary conditions)

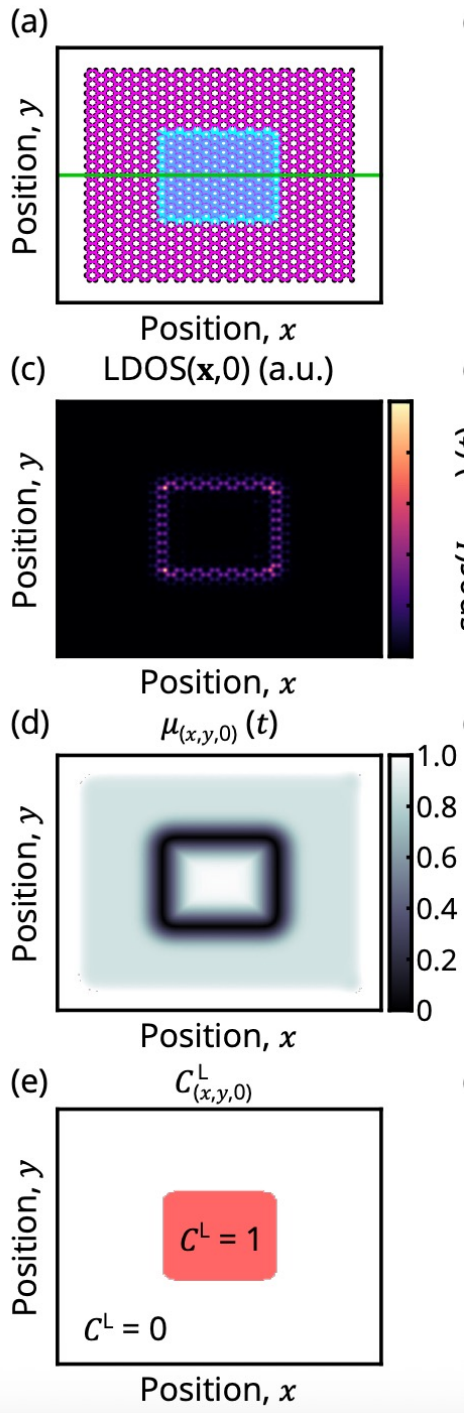
$$L(\mathbf{x}, E) = (\hat{X} - x) \otimes \sigma_x + (\hat{Y} - y) \otimes \sigma_y + (\hat{H} - E) \otimes \sigma_z$$

Local probe of topology resolved in position and energy

Chern marker defined through the signature:

$$C = \frac{1}{2} \operatorname{sgn} L(\mathbf{x}, E)$$

Generalizable to other symmetry classes



Kernel polynomial method

Need to solve large systems

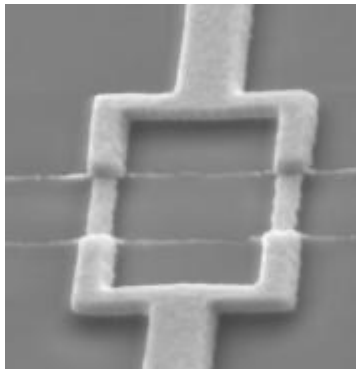
- Mesoscopic devices
- Bulk disordered materials

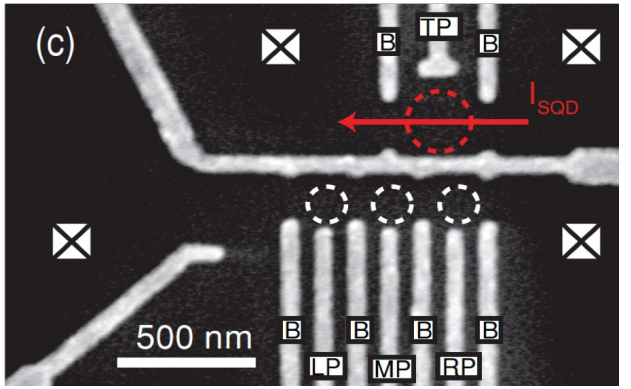
Computationally expensive

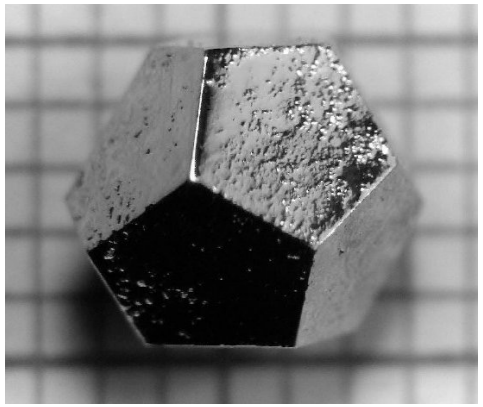
$O(N^3)$ scaling of diagonalization

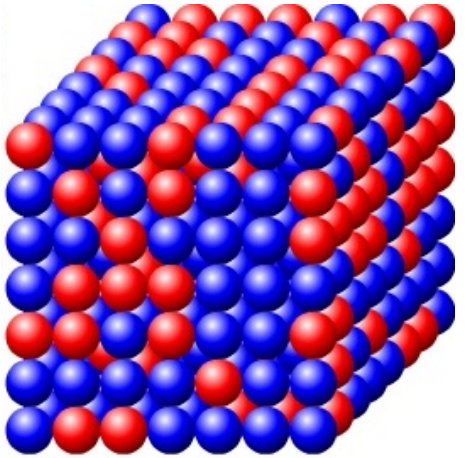
Interesting physics encoded in a few numbers

- Response functions
- Topological invariants









Symmetry				d							
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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

Kernel Polynomial Method

[Weiße et.al. Rev. Mod. Phys. **78**, 275 (2006)]

Orthogonal functions

$$\langle f|g\rangle_1 = \int_{-1}^{1} \frac{f(x)\,g(x)}{\pi\sqrt{1-x^2}}\,dx \qquad \langle T_n|T_m\rangle_1 = \frac{1+\delta_{n,0}}{2}\,\delta_{n,m}$$

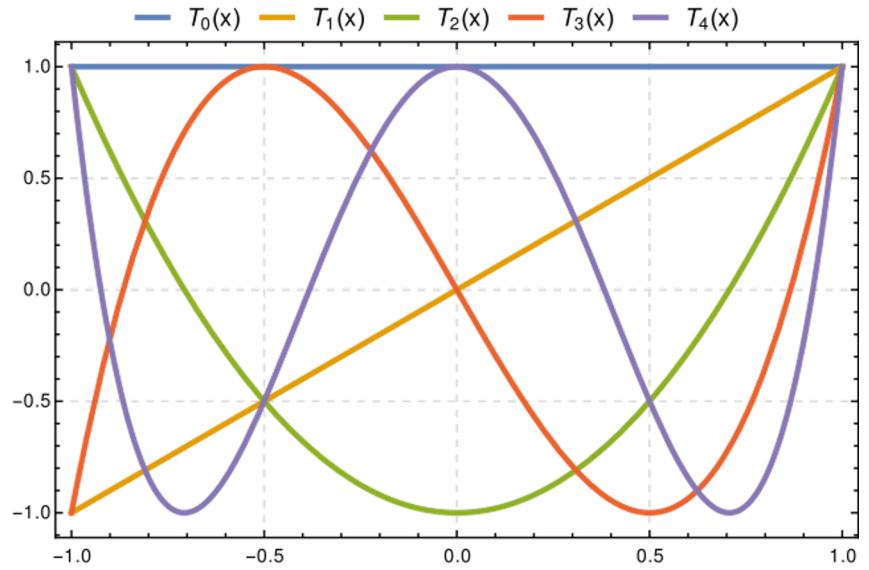
Expand function in Chebyshev polynomial basis

$$f(x) = \sum_{n=0}^{\infty} \frac{\langle f|T_n\rangle_1}{\langle T_n|T_n\rangle_1}\,T_n(x) = \alpha_0 + 2\sum_{n=1}^{\infty}\alpha_n\,T_n(x)$$

Can also include parameter dependence

Recursion relation

$$T_0(x) = 1\,, \quad T_{-1}(x) = T_1(x) = x\,,$$
$$T_{m+1}(x) = 2\,x\,T_m(x) - T_{m-1}(x)\,,$$



Kernel Polynomial Method

Evaluation of matrix functions

$$f(\hat{H},\lambda) \equiv \sum_k f(E_k,\lambda)|\psi_k\rangle\langle\psi_k|$$

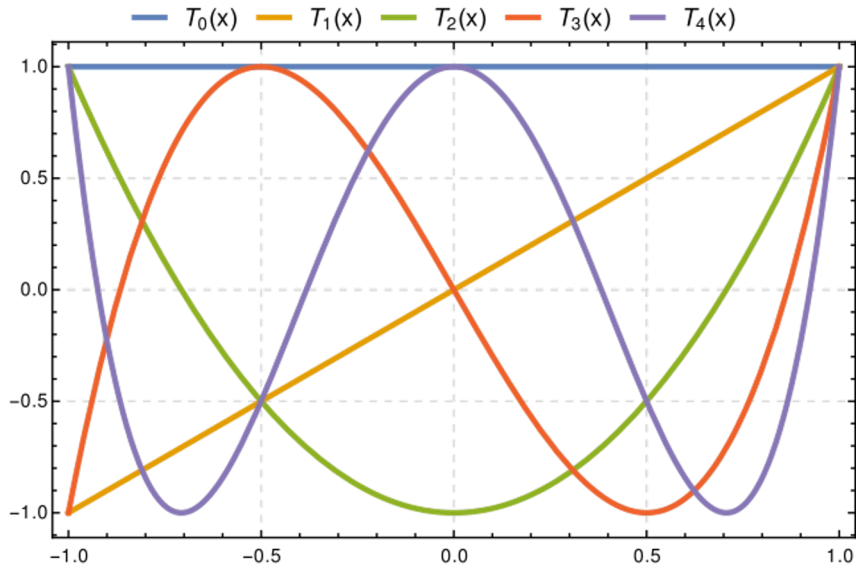
Expand function in Chebyshev polynomial basis

$$\tilde{f}(E,\lambda) = \sum_{m=0}^{M} \tilde{\alpha}_m(\lambda) T_m(E)$$

$$f(\hat{H},\lambda) \overset{\text{KPM}}{\approx} \tilde{f}(\hat{H},\lambda) \equiv \sum_k \tilde{f}(E_k,\lambda)|\psi_k\rangle\langle\psi_k|$$

Recursive evaluation of action on vector

Computational effort scales as $\mathrm{O}(MN)$



$$\begin{aligned} |v_0\rangle &= T_0(H)\,|v\rangle &&= |v\rangle \\ |v_1\rangle &= T_1(H)\,|v\rangle &&= H\,|v\rangle \\ |v_{n+1}\rangle &= T_{n+1}(H)\,|v\rangle &&= 2H\,|v_n\rangle - |v_{n-1}\rangle \end{aligned}$$

$$f(\hat{H},\lambda)|v\rangle \overset{\text{KPM}}{\approx} \sum_k \tilde{\alpha}(\lambda)|v_m\rangle$$

[Weiße et.al. Rev. Mod. Phys. **78**, 275 (2006)]

Kernel Polynomial Method

Operator expectation values

$$\langle \hat{A} \rangle_{E_F} = \sum_k f(E_k, E_F) \langle \psi_k | \hat{A} | \psi_k \rangle = \mathrm{Tr}\left(\hat{A}\, f(\hat{H}, E_F) \right)$$

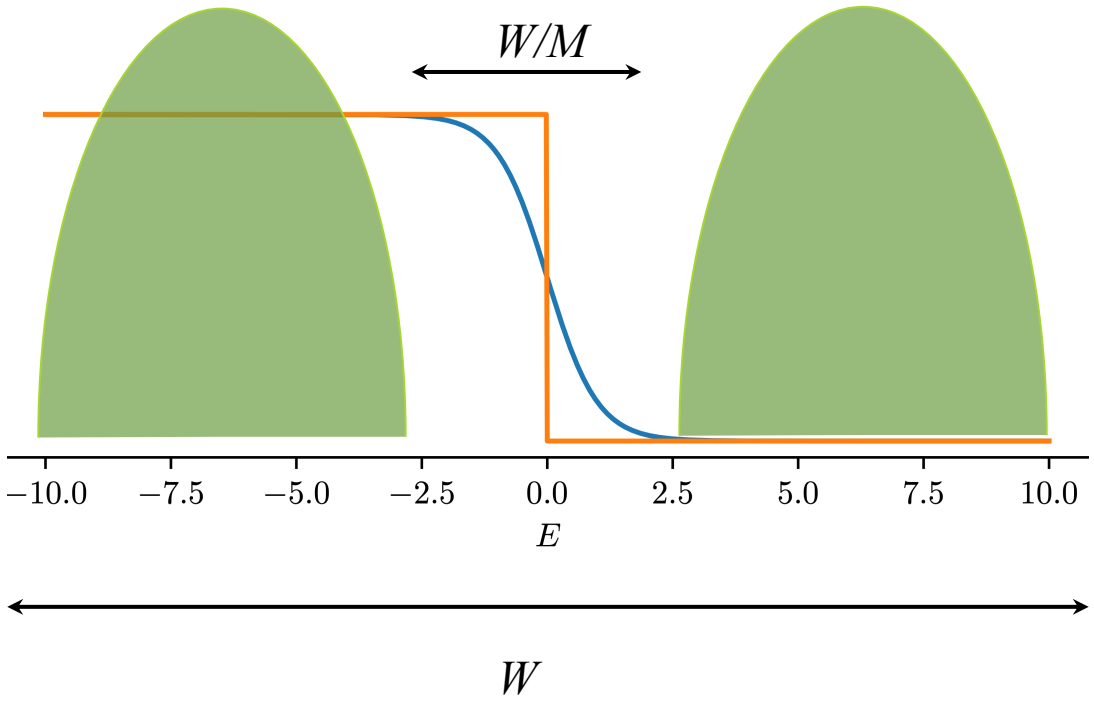
Spectral density $\rho(E) = \mathrm{Tr}\left(\delta(E - \hat{H}) \right)$

Trace estimated by stochastic trace

$$\mathrm{Tr}\left(\hat{A} \right) \approx \frac{1}{R} \sum_{r=1}^{R} \langle r | \hat{A} | r \rangle$$

The bigger the system the better it works

Resolution W/M given by number of modes M



[Weiße et.al. Rev. Mod. Phys. **78**, 275 (2006)]

Application: Mirror Chern insulator in 3D

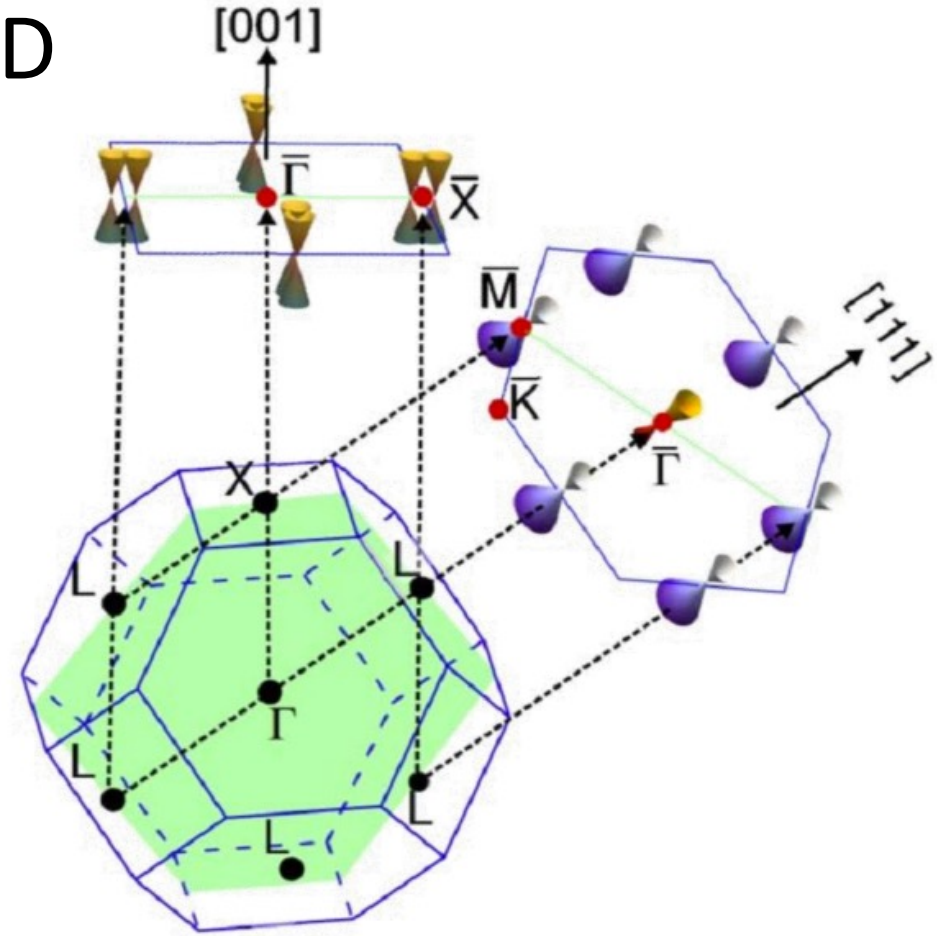
First topological crystalline phase

Requires mirror symmetry

Mirror even and odd states have separate Chern number

Mirror Chern number C_M

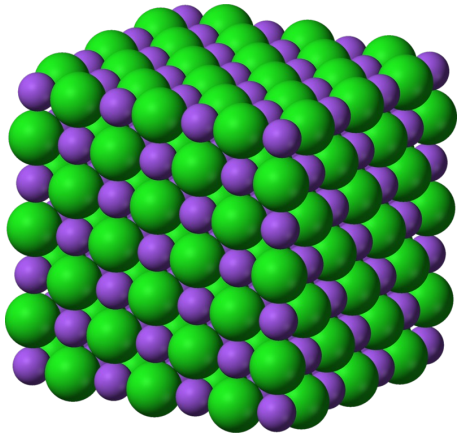
$$C_M = \frac{1}{2}(C_+ - C_-)$$

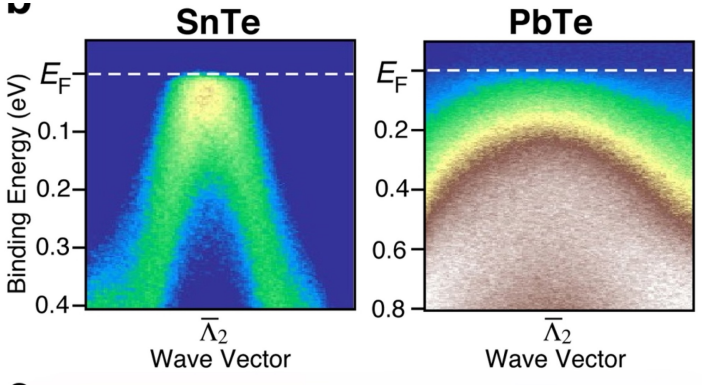


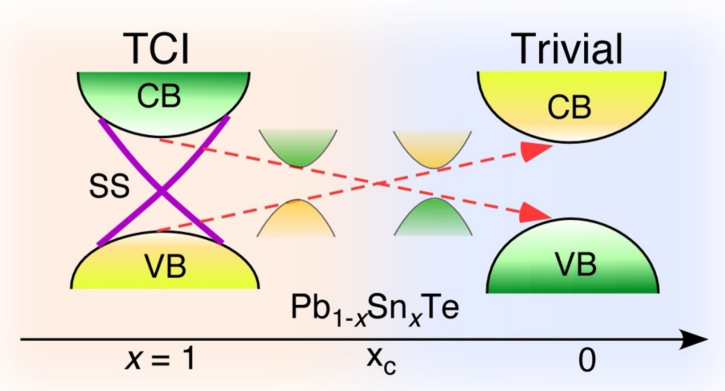
Hsieh et al. Nat. Commun. 3, 982 (2012)

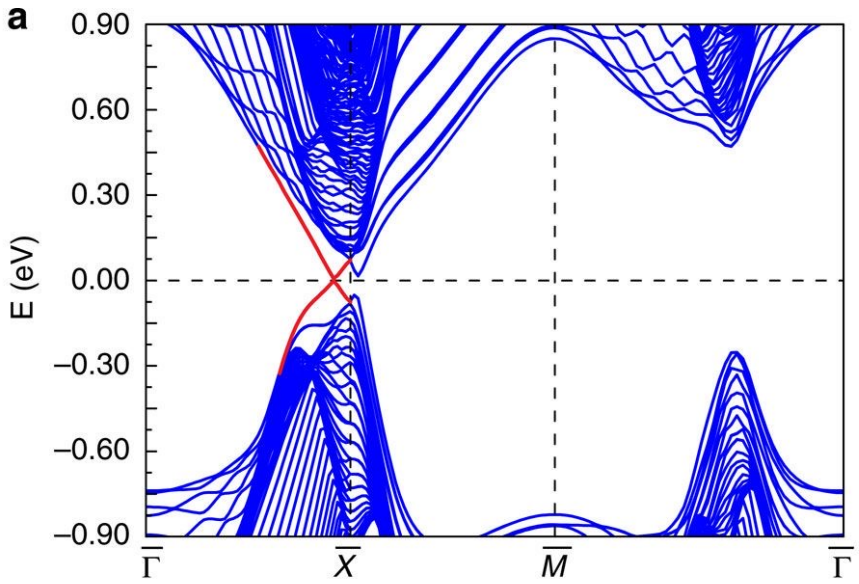
$Sn_xPb_{1-x}Te$

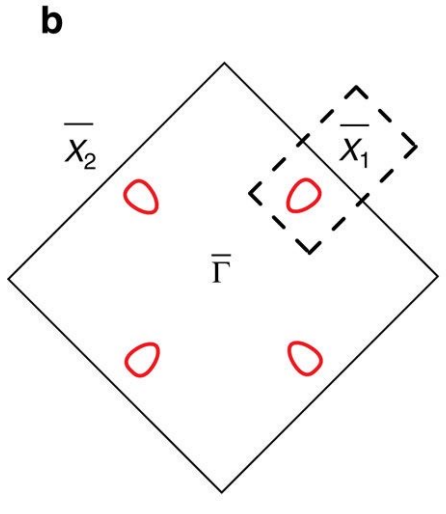
- Rocksalt structure
- Substitutional disorder
- Band inversion between PbTe and SnTe
- Studied using virtual crystal approximation

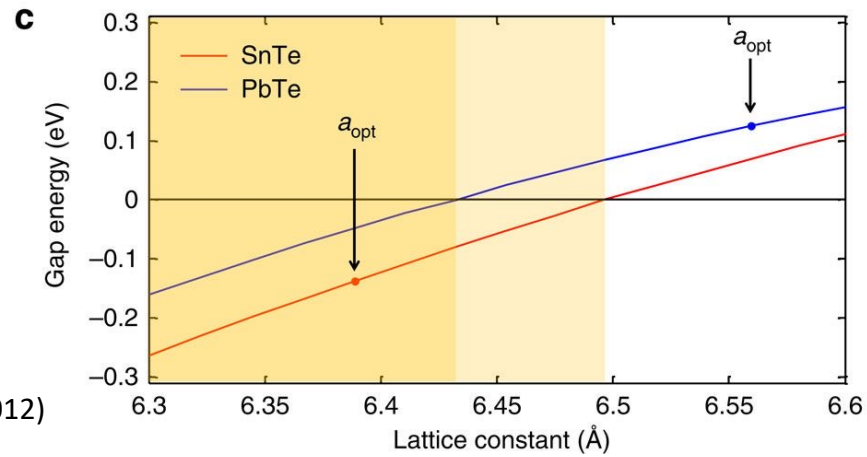








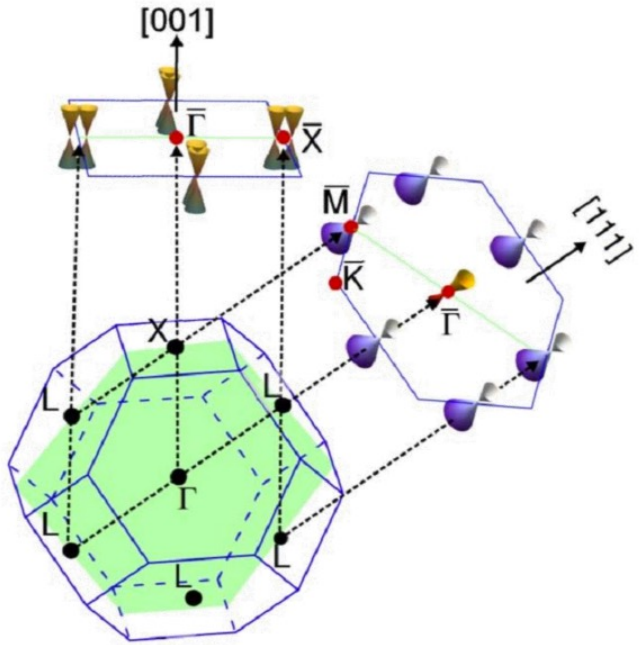




Hsieh et al. Nat. Commun. 3, 982 (2012)
Tanaka et al. Nature Physics, *8*(11), 800 (2012)

Disordered mirror Chern insulator

How to calculate invariant with disorder?



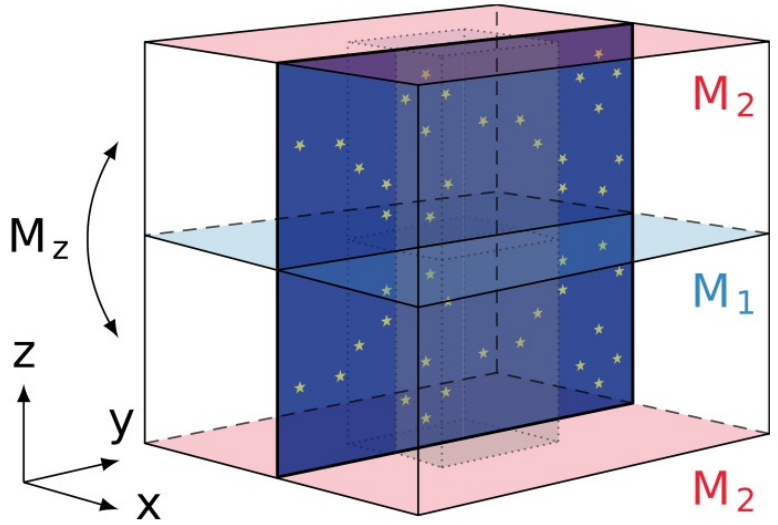
Previous best method was the scattering matrix invariant [Fulga et al. PRB **85**, 165409 (2012)]

$$\mathcal{O}\left(\xi^{3(d-1)}\right)$$

KPM mirror Chern number

$$\mathcal{O}\left(\xi^{d+1}\right) \qquad C_M = -\frac{\pi i}{A}\mathrm{Tr}_A\left(M_z\left[\hat{X},\hat{Y}\right]\right)$$

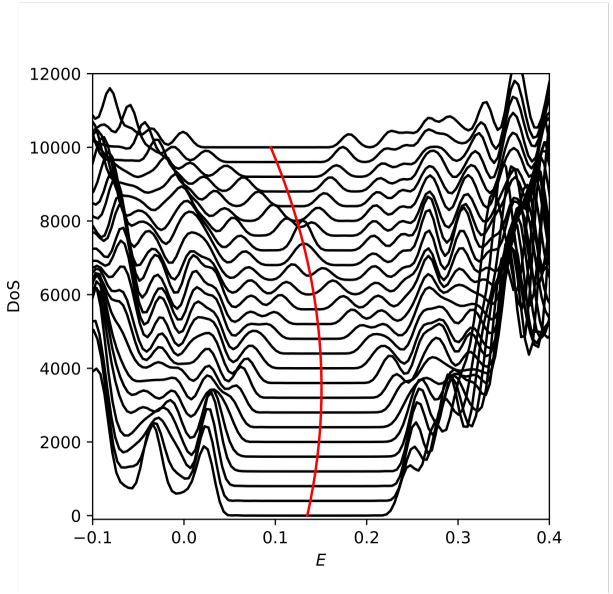
$L \cong \xi \cong 100$ sites



Results for $Sn_xPb_{1-x}Te$

[Varjas, Akhmerov, Pérez-Piskunow, Fruchart, Phys. Rev. Research **2**, 013229 (2020)]

- First study using realistic model: spinful s, p, d orbitals
- More accurate than previous studies using VCA

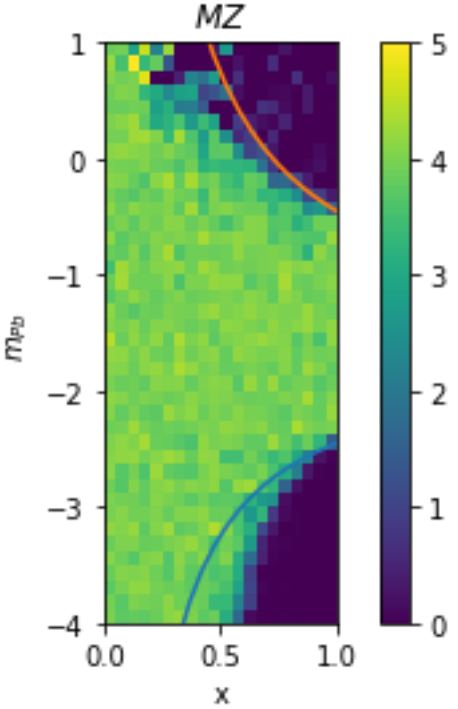


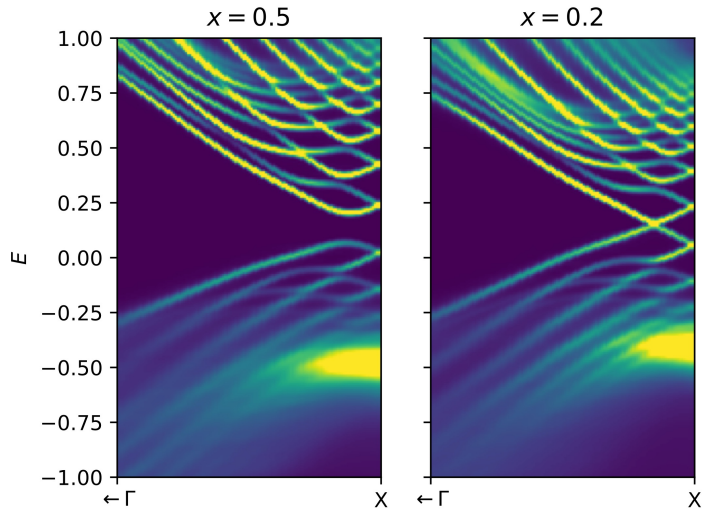
$Sn_{1-x}A_xTe$

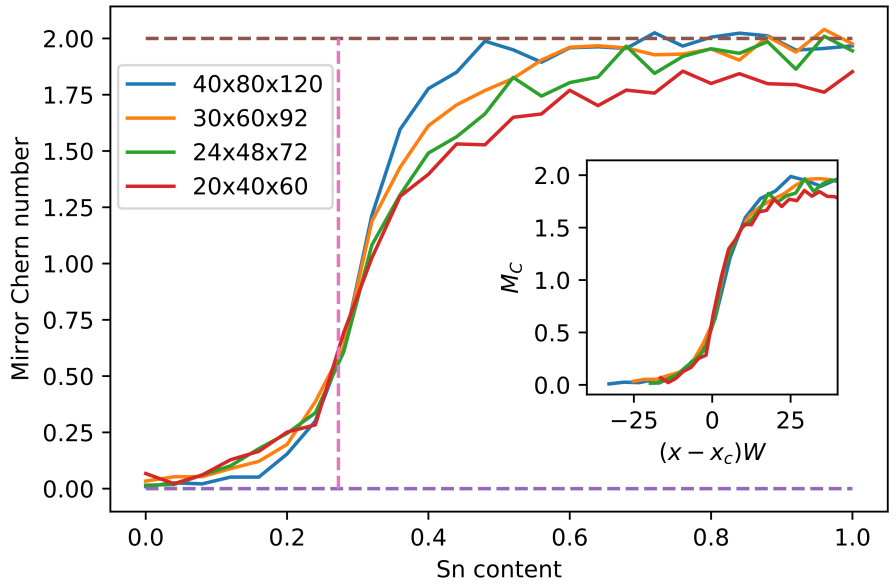
Ge

Sn

Pb

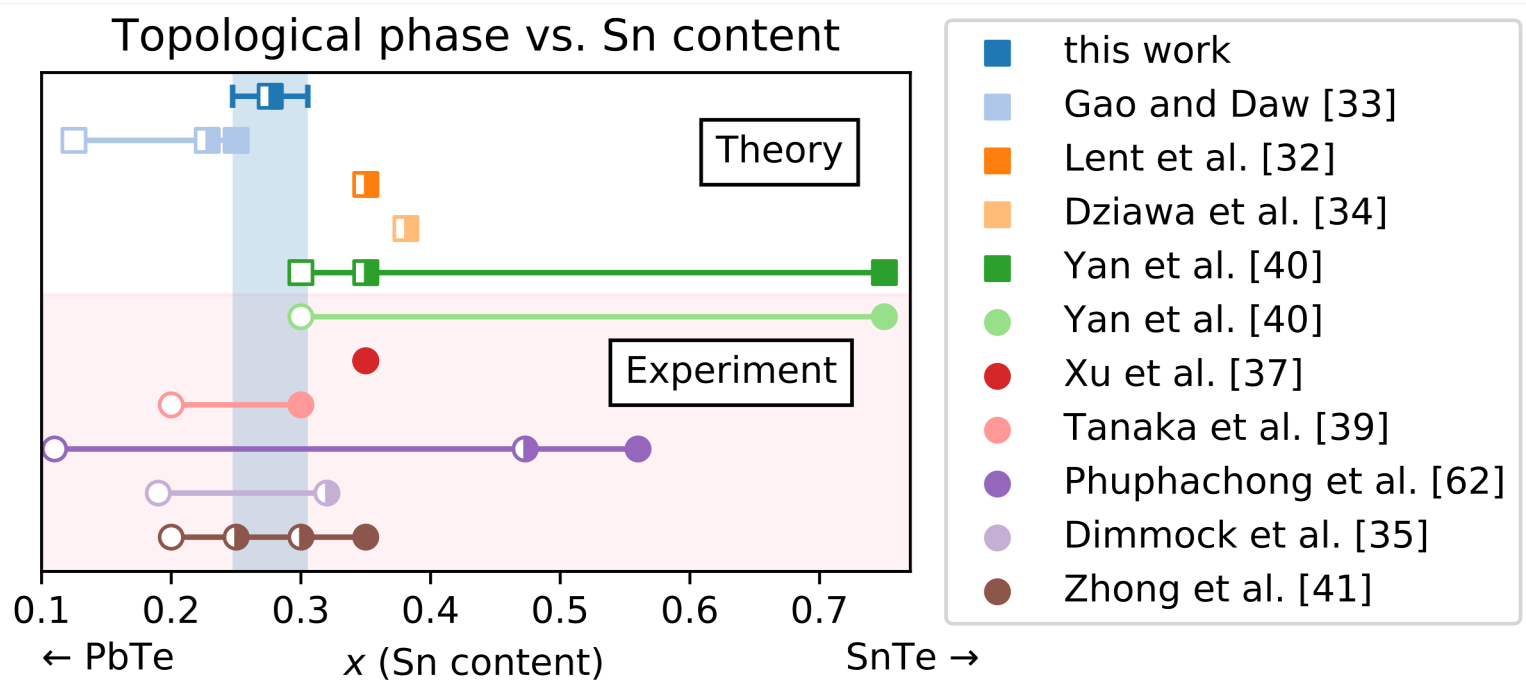


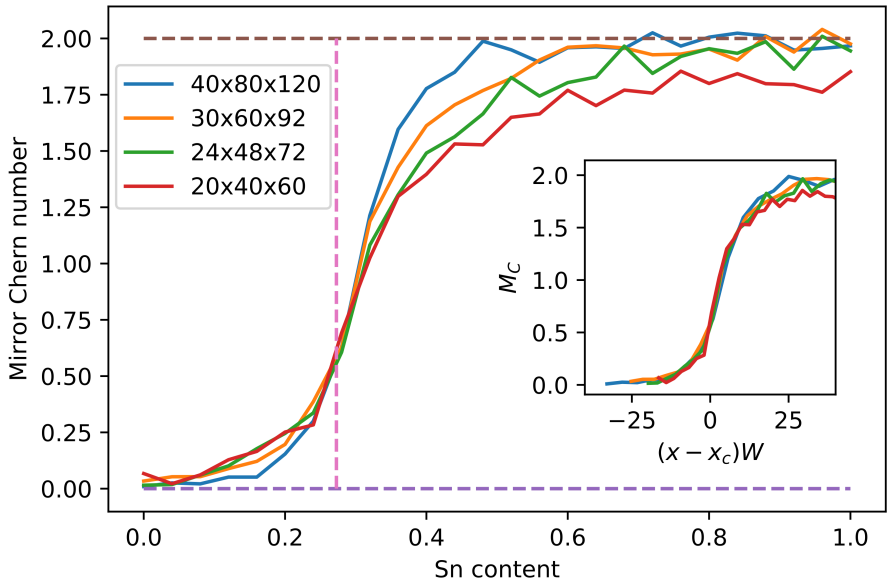




Results for $Sn_xPb_{1-x}Te$

- More accurate than previous studies using VCA
- Agrees with available experimental data
- Good news for experiments and fabrication
- Can be improved using DFT data for disordered clusters





Real space Topological Markers in other symmetry classes

- Similar formulation for all Z invariants
- Best speed advantage in 3D
- Disordered topological superconductor (class DIII)