Real-space screening of bulk topology of high-quality two-dimensional insulators

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Outline

- Can real-space topological response be used to scan and predict bulk topology of realistic models of quantum materials?

- Magnetic flux tube: spin-charge separation for 2D quantum spin Hall states with and without gapless edge states

- Flux tube-based screening of 2D materials database: large band gap topological insulators which are not predicted by symmetry indicators

- Summary

Relevant papers

(1) A. Tyner et al., Topology of three-dimensional Dirac semimetals and generalized quantum spin Hall systems without gapless edge modes (arXiv:2012.12906) [Phys. Rev. Research **5**, L012019, (2023)]

(2) A. Tyner and P. Goswami, Spin-charge separation and quantum spin Hall effect of beta-bismuthine, arXiv:2209.13582 (to be published in Scientific Reports)

(3) A. Tyner and P. Goswami, Solitons and real-space screening of bulk topology of quantum materials, arXiv:2304.05424

Altland-Zirnbauer classification scheme

Three global discrete symmetries:

(1) time reversal (T),
(2) charge conjugation (C)
(3) chiral or sublattice (S)

Spin-orbit coupled, non-magnetic, non-superconducting materials: class AII

class\\δ	T	C	S	0	1	2	3	4	5	6	7
A	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII	0	0	1	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI	+	0	0	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
BDI	+	+	1	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
D	0	+	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
DIII	−	+	1	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
AII	−	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
CII	−	−	1	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
C	0	−	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
CI	+	−	1	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

Chiu et al., RMP 88, 035005 (2016)

Altland-Zirnbauer classification scheme

AZ Class	Symmetry group	$d=1$	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$	$d=7$	$d=8$
A	$U(1)$	$\mathbb{Z}$	$\mathbb{Z}^2$	$\mathbb{Z}$	$\mathbb{Z}^2$	$\mathbb{Z}$	$\mathbb{Z}^2$	$\mathbb{Z}$	$\mathbb{Z}^2$
AIII	$U(1)_{spin} \times Z_2^T$	0	0	0	0	0	0	0	0
AI	$U(1) \rtimes Z_2^T$ $(T^2=+1)$	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}^2$	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}^2$
BDI	Z_2^T $(T^2=+1)$	$\mathbb{Z}_2$	0	0	0	0	0	$\mathbb{Z}_2$	$(\mathbb{Z}_2)^2$
D	Z_2^f=N/A	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	$\mathbb{Z}_2$	$(\mathbb{Z}_2)^2$
DIII	Z_2^T $(T^2=-1)$	0	0	0	0	0	0	0	0
AII	$U(1) \rtimes Z_2^T$ $(T^2=-1)$	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}^2$	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}^2$
CII	$SU(2) \times Z_2^T$ $(T^2=+1)$	0	0	$\mathbb{Z}_2$	$(\mathbb{Z}_2)^2$	$\mathbb{Z}_2$	0	0	0
C	$SU(2)_{spin}$	0	$\mathbb{Z}$	$\mathbb{Z}_2$	$(\mathbb{Z}_2)^2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	$SU(2)_{spin} \times Z_2^T$ $(T^2=-1)$	0	0	0	0	0	0	0	0

Consideration of spatial discrete symmetries: new classes of topological crystalline insulators

Effects of space inversion symmetry:

(Lu and Lee, arXiv:1403.5558)

Non-trivial systems may not support gapless surface states

Reflection/mirror symmetry

Chiu et al., RMP 88, 035005 (2016)

protected, gapless surface states

Reflection	TCI/TCS	d=1	d=2	d=3	d=4
	FS1 in mirror	p=8	p=1	p=2	p=3
	FS2 in mirror	p=2	p=3	p=4	p=5
R	A	$M\mathbb{Z}$	0	$M\mathbb{Z}$	0
R_+	AIII	0	$M\mathbb{Z}$	0	$M\mathbb{Z}$
R_-	AIII	$M\mathbb{Z}\oplus\mathbb{Z}$	0	$M\mathbb{Z}\oplus\mathbb{Z}$	0
R_+, R_{++}	AI	$M\mathbb{Z}$	0	0^a	0
	BDI	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0	0^a
	D	$M\mathbb{Z}_2^a$	$M\mathbb{Z}_2$	$M\mathbb{Z}$	0
	DIII	0	$M\mathbb{Z}_2^a$	$M\mathbb{Z}_2$	$M\mathbb{Z}$
	AII	$2M\mathbb{Z}^a$	0	$M\mathbb{Z}_2^a$	$M\mathbb{Z}_2$
	CII	0	$2M\mathbb{Z}^a$	0	$M\mathbb{Z}_2^a$
	C	0^a	0	$2M\mathbb{Z}^a$	0
	CI	0	0^a	0	$2M\mathbb{Z}^a$
R_-, R_{--}	AI	0^a	0	$2M\mathbb{Z}^a$	0
	BDI	0	0^a	0	$2M\mathbb{Z}^a$
	D	$M\mathbb{Z}$	0	0^a	0
	DIII	$\mathbb{Z}_2$	$M\mathbb{Z}$	0	0^a
	AII	$T\mathbb{Z}_2^a$	$\mathbb{Z}_2$	$M\mathbb{Z}$	0
	CII	0	$T\mathbb{Z}_2^a$	$\mathbb{Z}_2$	$M\mathbb{Z}$
	C	$2M\mathbb{Z}^a$	0	$T\mathbb{Z}_2^a$	$\mathbb{Z}_2$
	CI	0	$2M\mathbb{Z}^a$	0	$T\mathbb{Z}_2^a$

High throughput screening of band topology

- realistic models of materials: symmetry-based indicators + Wilson loop spectrum

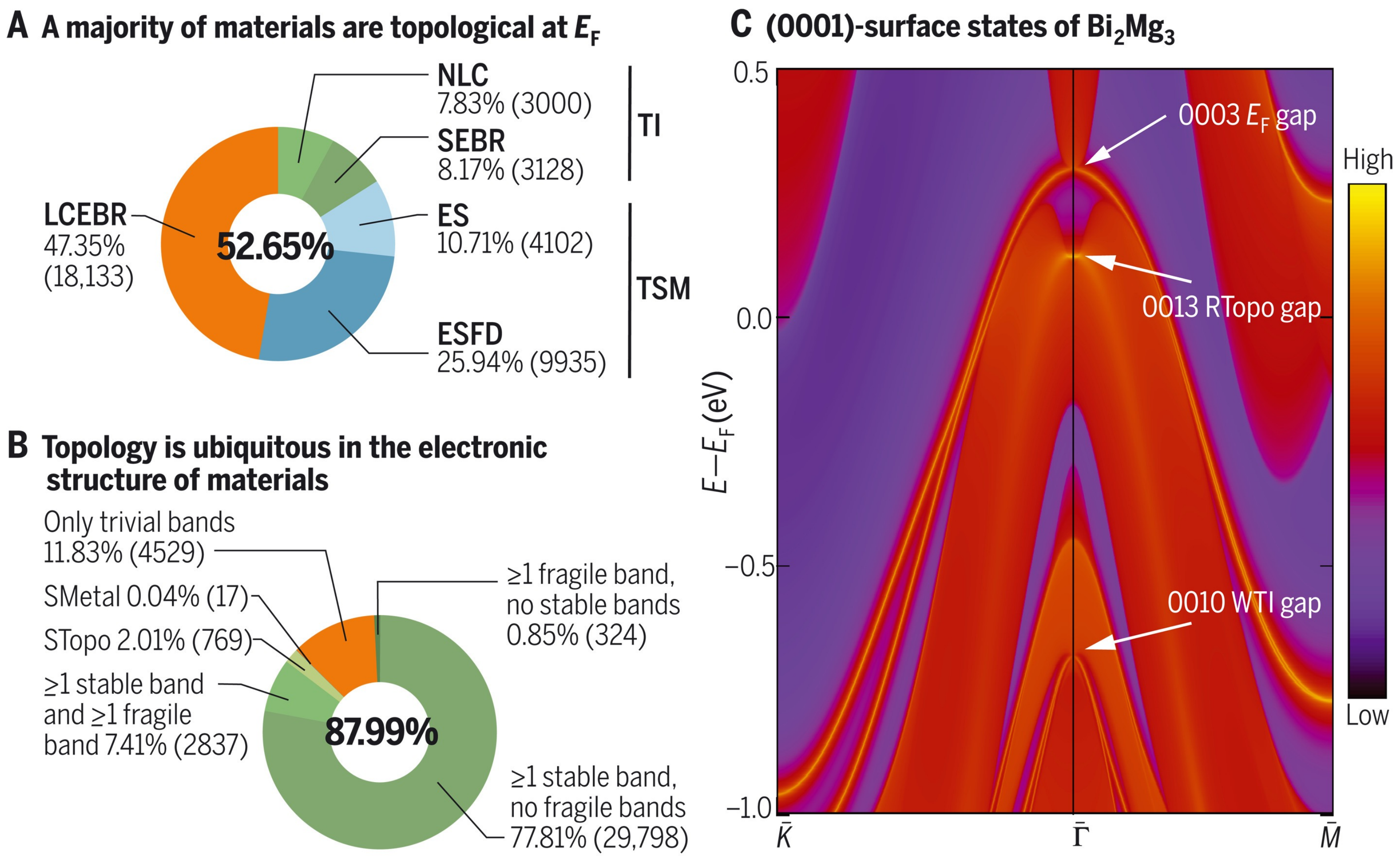


Fig. from: Vergniory et. al, Science, Vol 376, Issue 6595, (2022)

What are the physical significance of new invariants and phases?

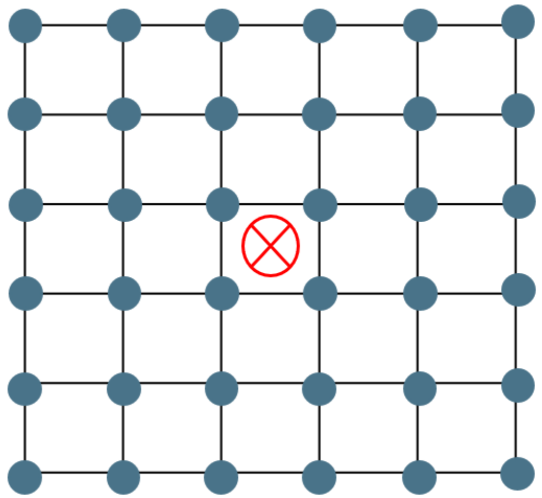
How to detect topology beyond symmetry indicators?

Spin-charge separation for QSH state

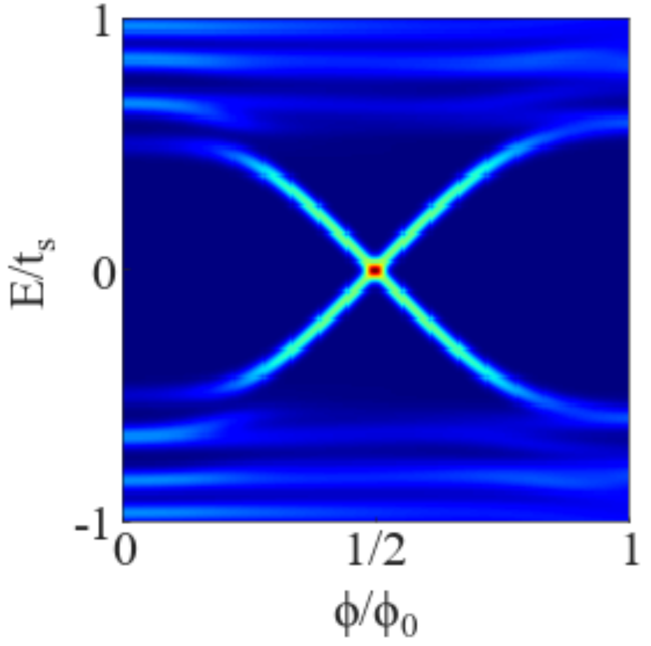
$$H(\mathbf{k}) = t_p \sin k_x \Gamma_1 + t_p \sin k_y \Gamma_2 + t_s(\Delta - \cos k_x - \cos k_y)\Gamma_3$$

BHZ model: two copies of quantum Hall; cross-correlated charge and spin response

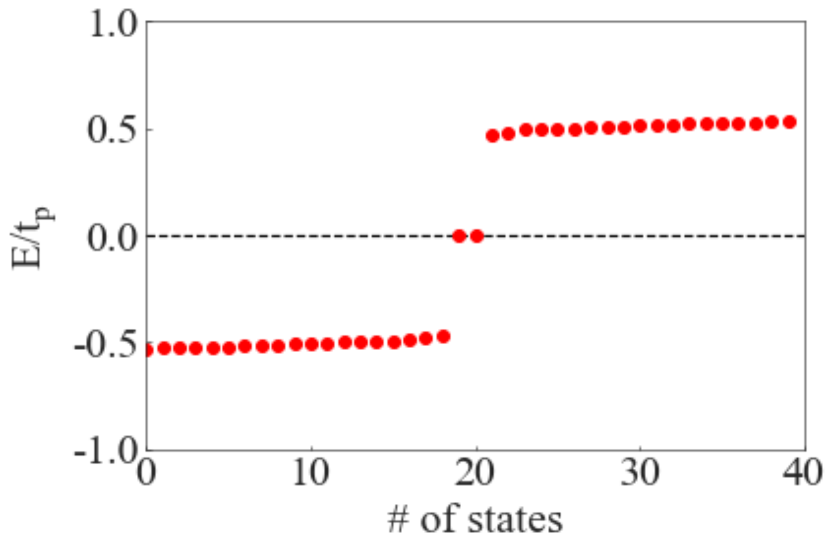
Magnetic pi-flux tube leads to spin-charge separation (Qi & Zhang, PRL 101, 086802 (2008); Ran et al, PRL 101, 086801 (2008))



for systems without gapless edge states:Tyner et. al, arXiv:2012.12906 (PRR)



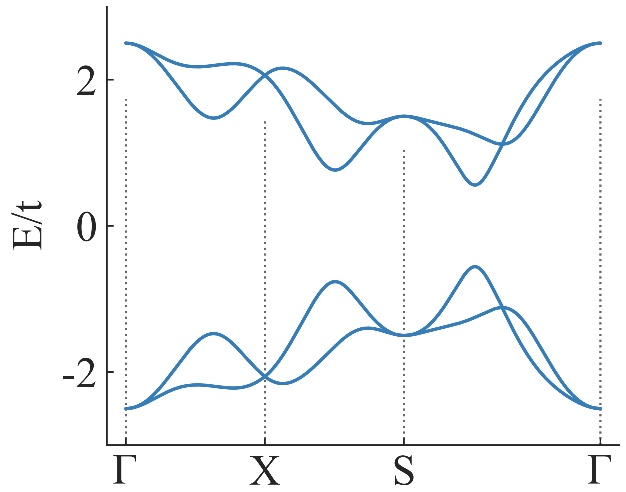
LDOS on vortex



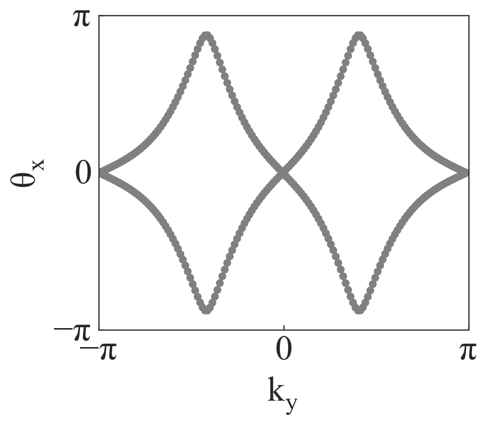
Kramers doublet for π-flux

Spin-charge separation for even integer QSH state

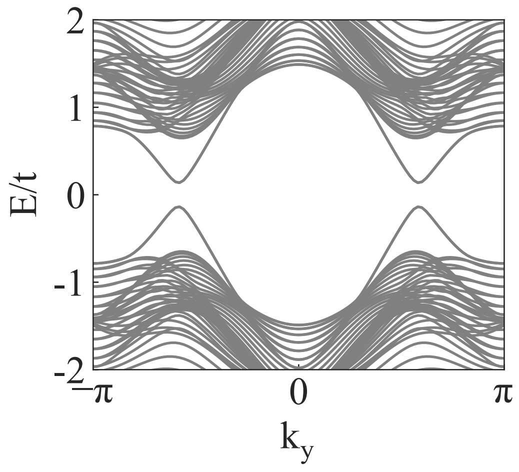
$$\begin{aligned}H(\mathbf{k}) = &\, 2t_2(\sin k_x \sin k_y)\sigma_0 \otimes \tau_1 \\ &+ t_1(\cos k_x - \cos k_y)\sigma_3 \otimes \tau_2 \\ &+ (t_1' + 2t_2'(\cos k_x + \cos k_y) - 2t)\sigma_0 \otimes \tau_3 \\ &+ t_3(\cos 2k_x - \cos 2k_y)\sigma_2 \otimes \tau_2 + \\ &0.5t_4\left(\sin k_x \cos k_y + \sin k_y \cos k_x\right)\sigma_1 \otimes \tau_1\end{aligned}$$



(band structure)

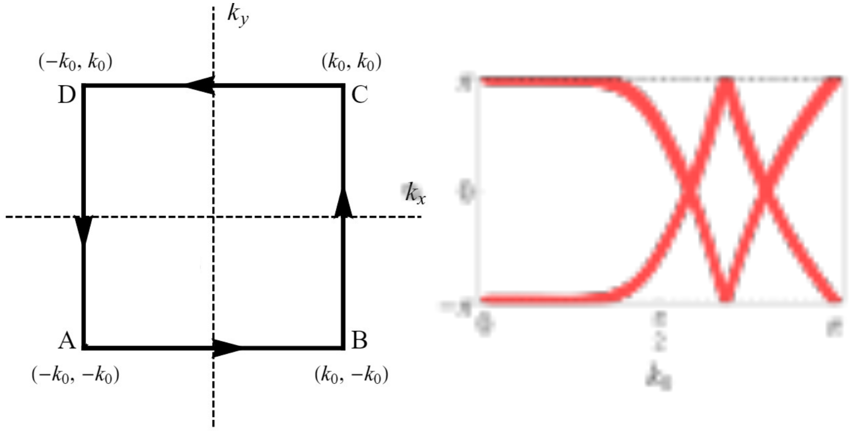


(b)



(c)

Gapped Wannier charge centers;
gapped edge states

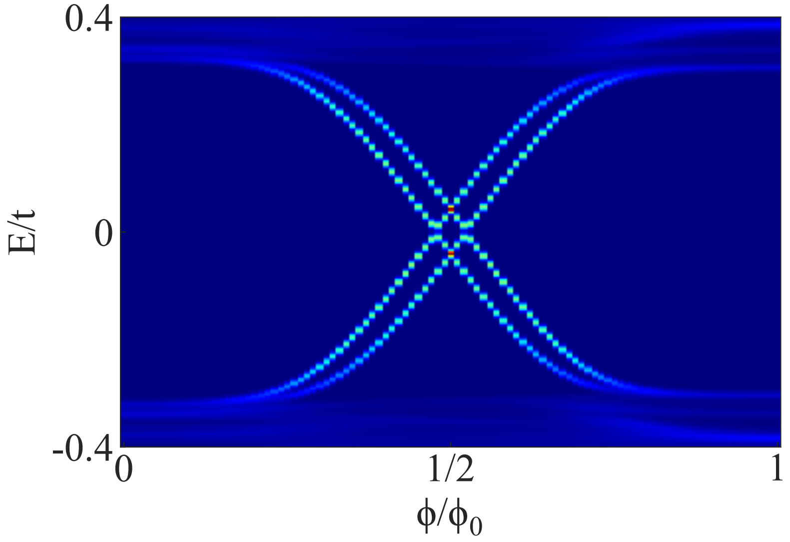


(winding of in plane Wilson loop spectrum)

(Tyner & Goswami, arXiv:2304.05424)

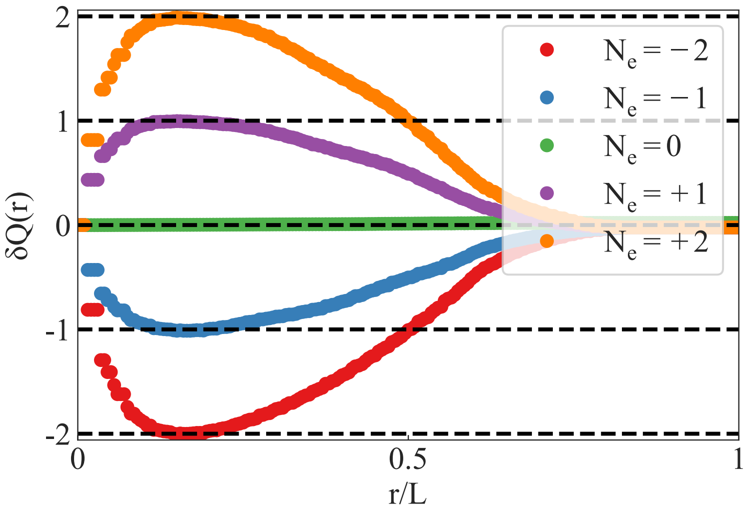
Spin-charge separation for even integer QSH state

4 mid-gap modes for pi flux tube: splitting of two doublets for BHZ type model with U(1) spin-rotation symmetry



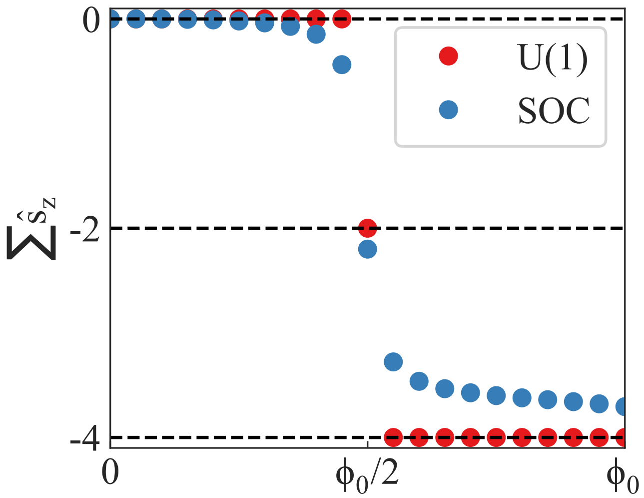
(g)

Spectrum for magnetic flux tube



(h)

Induced electric charge away from half-filling



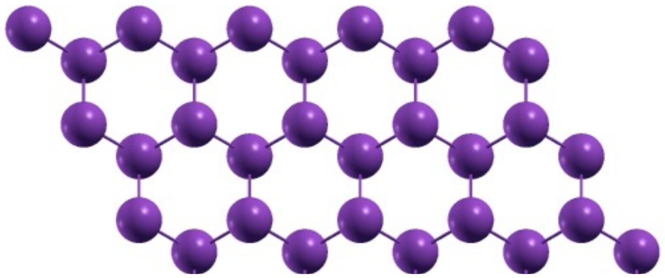
Induced spin polarization at half-filling

(Tyner & Goswami, arXiv:2304.05424)

First-principles integration

- Flux tube calculation for DFT derived models of bilayer bismuth (β-bismuthene)
- Classified as QSH insulator

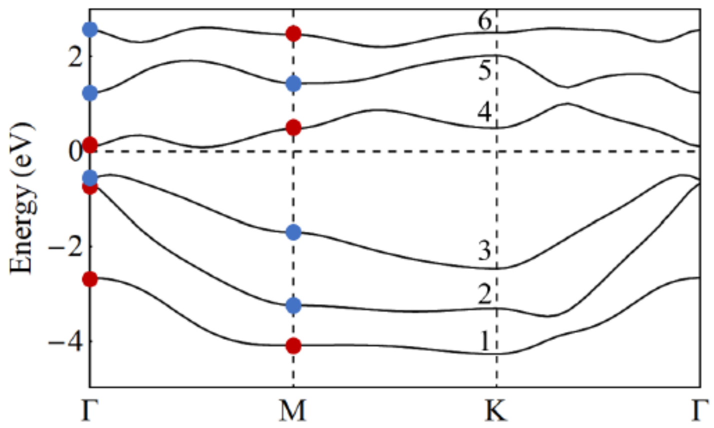
Phys. Rev. Lett. 97, 236805, (2006)
Phys. Rev. B. 83, 121310(R), (2011)

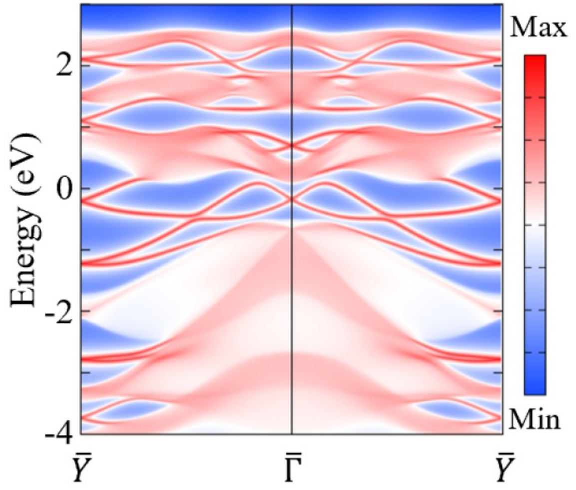


Bilayer bismuth (β-bismuthene)

Tyner & Goswami, arXiv:2209.13582

$\nu = +1$

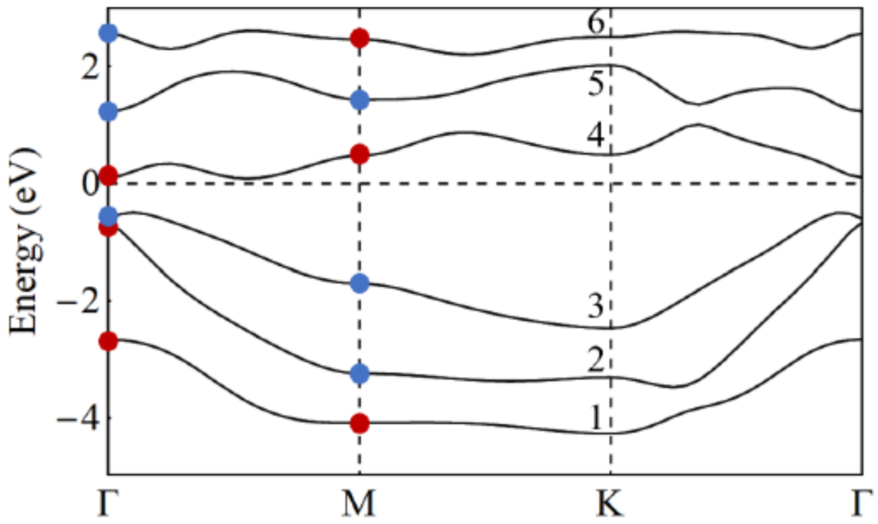




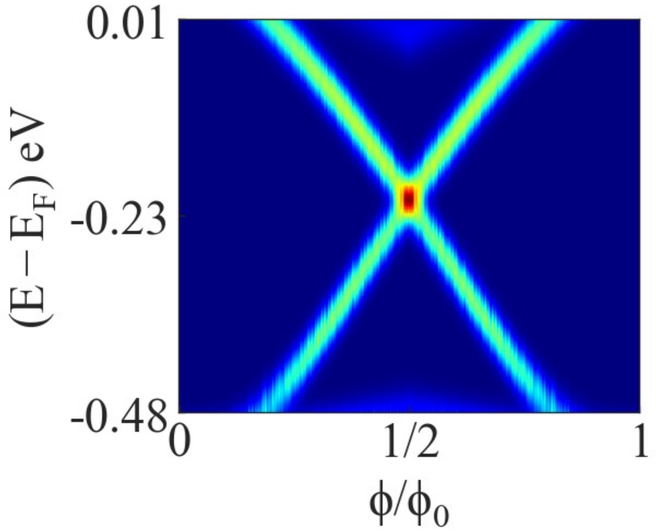
Spin Chern number $C_s = \pm 1, \ \pm 3?$

First-principles integration

- Developed software to perform vortex insertion for DFT derived models



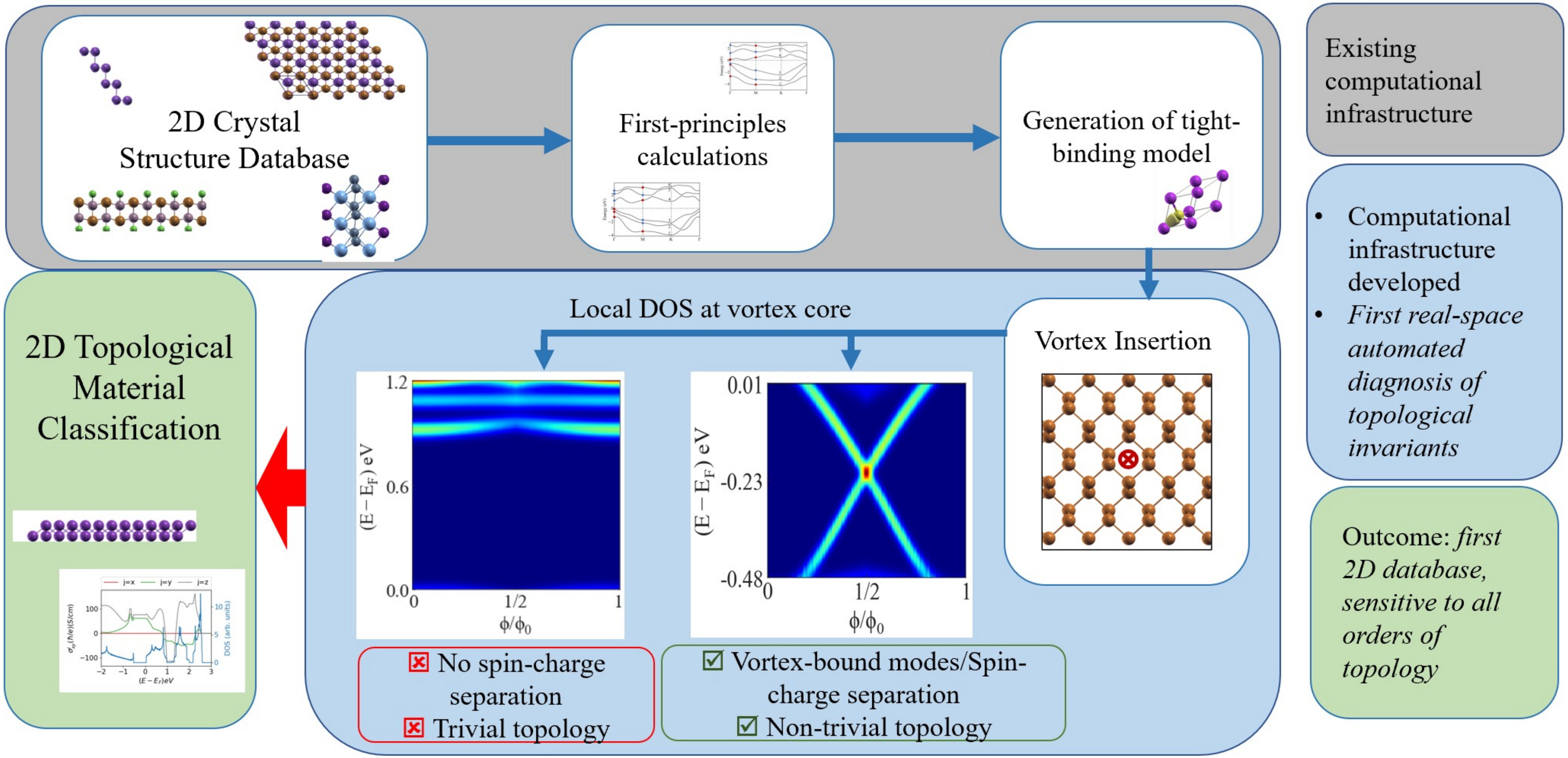
Tyner & Goswami,
arXiv:2209.13582



$$|C_s| = 1$$

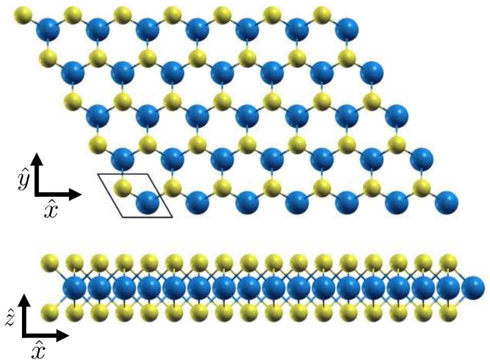
First-principles integration

(Tyner & Goswami, arXiv:2304.05424)

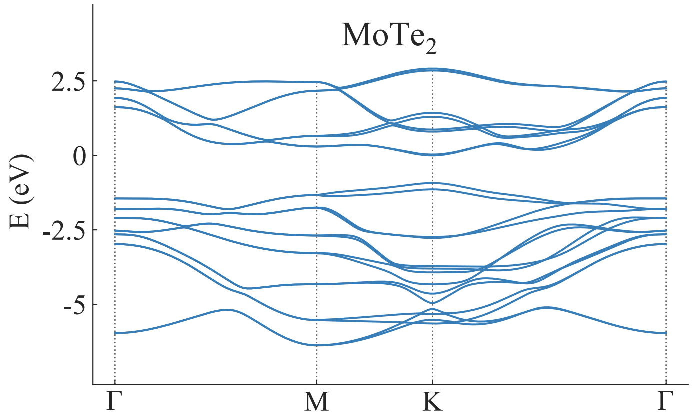


First-principles integration

- Monolayer 1H TMDs
- Z_2-trivial, large band gap, insulator



(a)



(b)

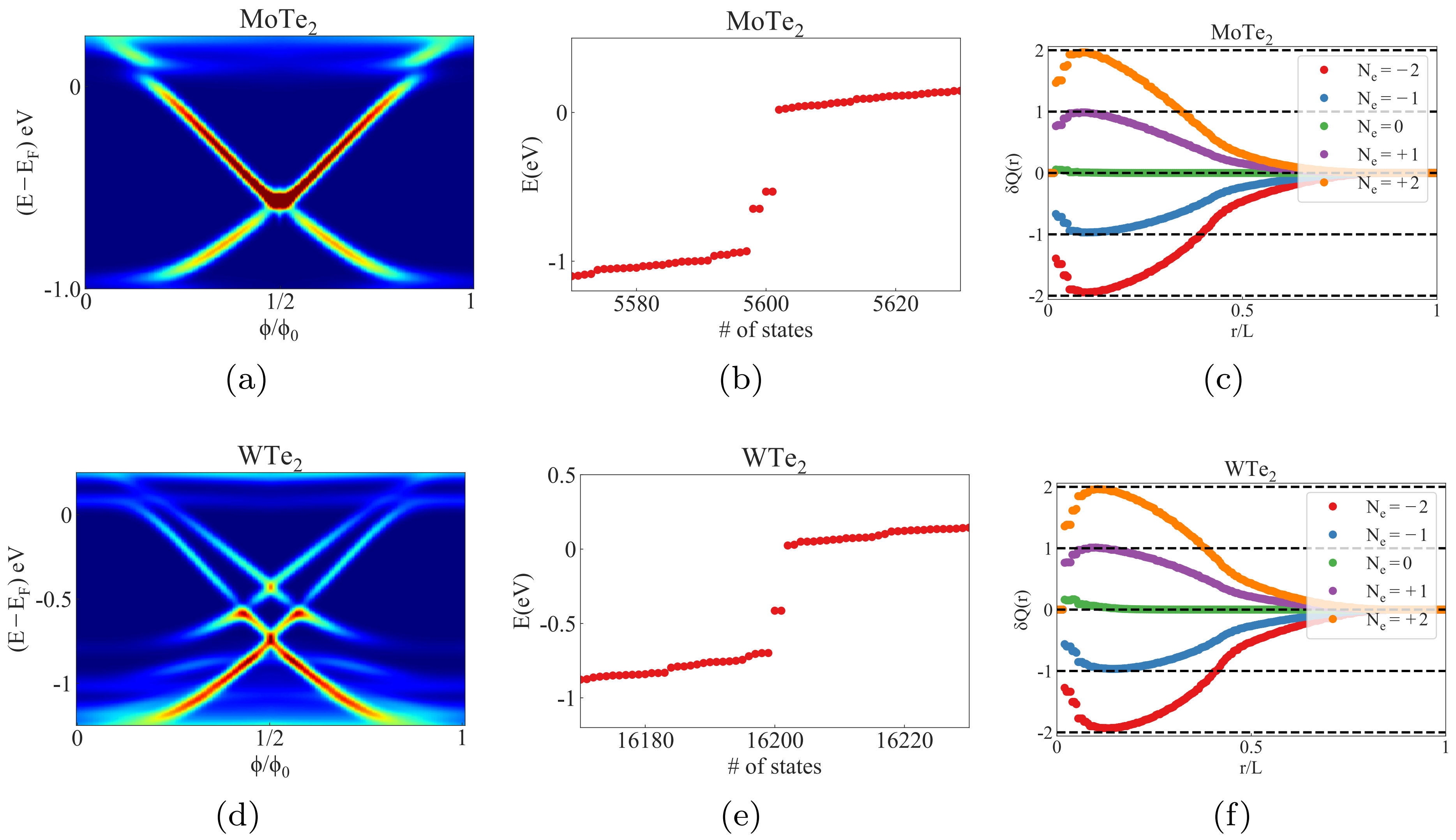
(Tyner & Goswami, arXiv:2304.05424)

	ΔE_{DFT}
$MoTe_2$	1.1 eV
MoS_2	1.6 eV
$MoSe_2$	1.5 eV
WSe_2	1.6 eV
WS_2	1.8 eV
WTe_2	1.1 eV

(c)

First-principles integration

Probing with flux tube (Tyner & Goswami, arXiv:2304.05424)

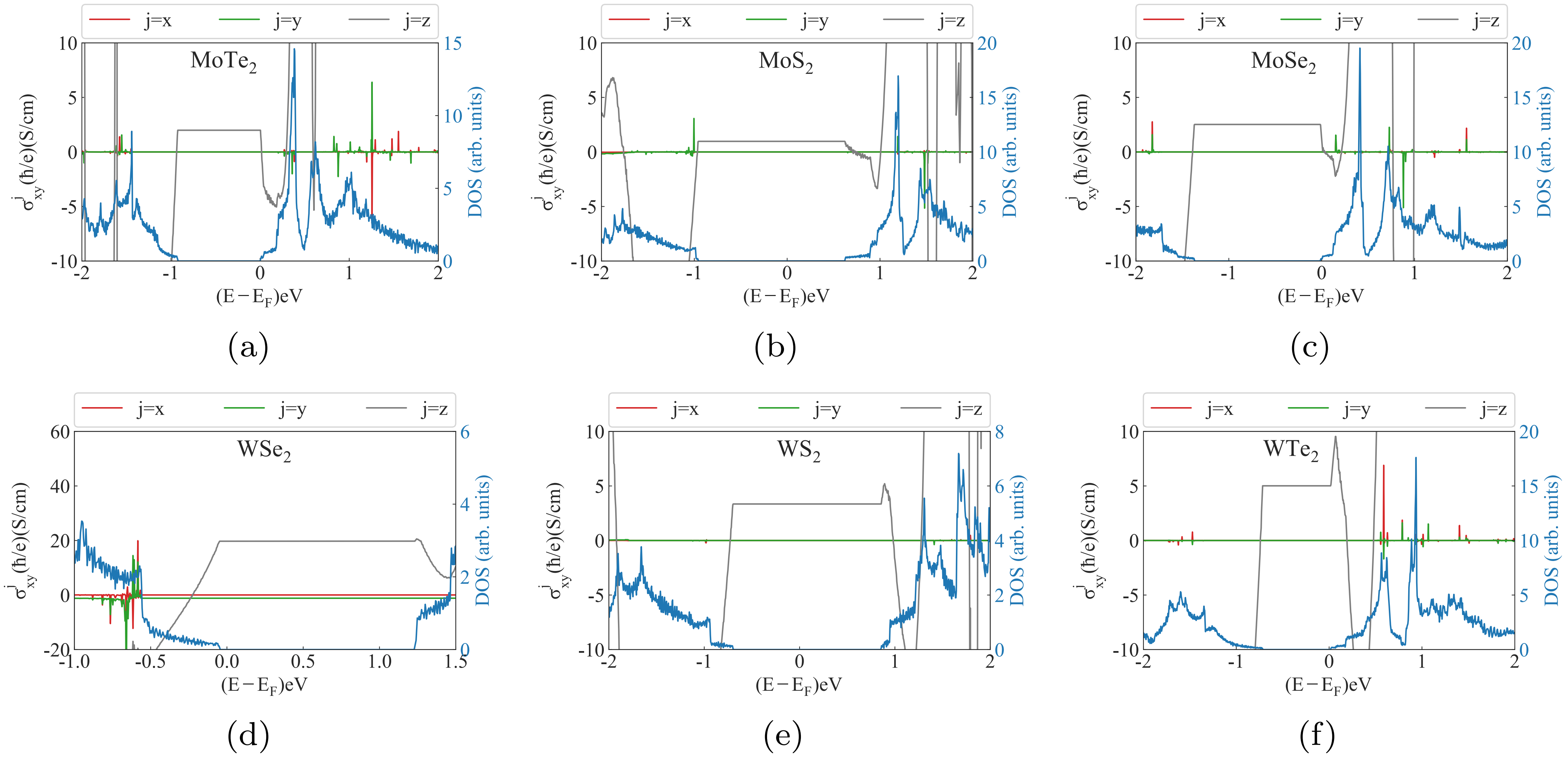


Formula	Spacegroup	Band gap (eV)	Z2 Index	|Cs,G|
Au2Br2	Cmme	2	0	2
Bi2	P-3m1	0.6	1	1
CdI2	P-3m1	2.4	0	2
Cu2I2	P-3m1	2	0	2
FeCl2	P-3m1	0.9	0	2
GeI2	P-3m1	2.1	0	2
GeI2	P-6m2	2	0	2
MoS2	P-6m2	1.6	0	2
MoSe2	P-6m2	1.5	0	2
MoTe2	P-6m2	1.1	0	2
NiO2	P-3m1	1.3	0	2
PtO2	P-3m1	1.7	0	2
PtS2	P-3m1	1.8	0	2
PtSe2	P-3m1	1.3	0	2
Sn2O2	P4/nmm	3	0	2
Tl2S	P-3m1	1.4	0	2
WS2	P-6m2	1.8	0	2
WSe2	P-6m2	1.6	0	2
WTe2	P-6m2	1.1	0	2
ZnCl2	P-3m1	4.5	0	2
ZnCl2	P-4m2	4.3	0	2
ZrCl2	P-6m2	1	0	2

higher-order, quantum spin Hall insulators with even integer spin Chern number

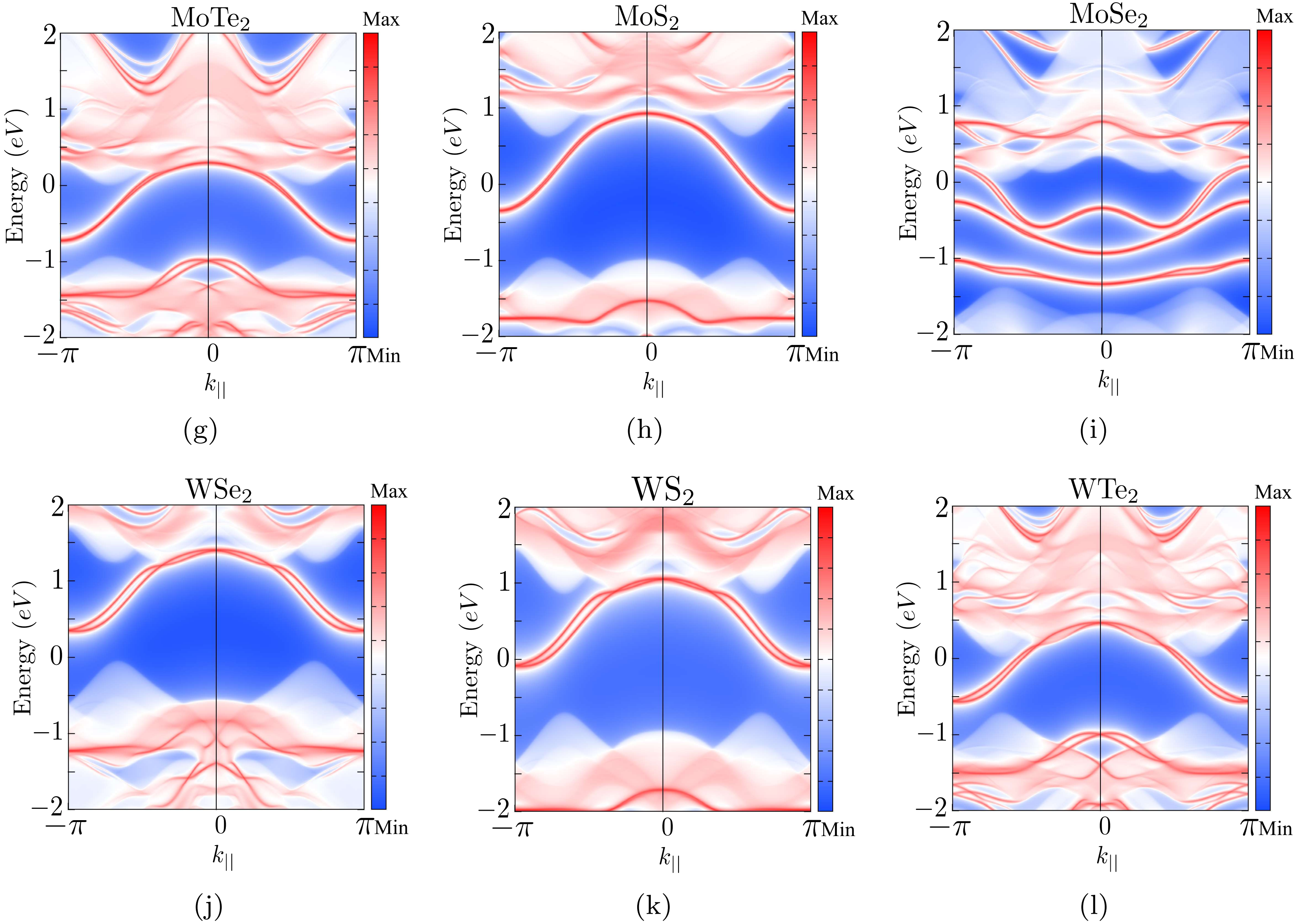
(Tyner & Goswami, arXiv:2304.05424)

Calculation of spin Hall conductivity (WannierBeri)



(Tyner & Goswami, arXiv:2304.05424)

Edge spectrum (not fully connected)



(Tyner & Goswami, arXiv:2304.05424)

Summary

- Magnetic-flux tube: non-perturbative probe to predict spin Chern number regardless of the presence of additional symmetries or gapless edge states

- Real-space probes are ideally suited for quasi-crystals, disordered, and correlated systems

- New experiments on 1H TMDs and closely related large band gap materials?

Thank you!