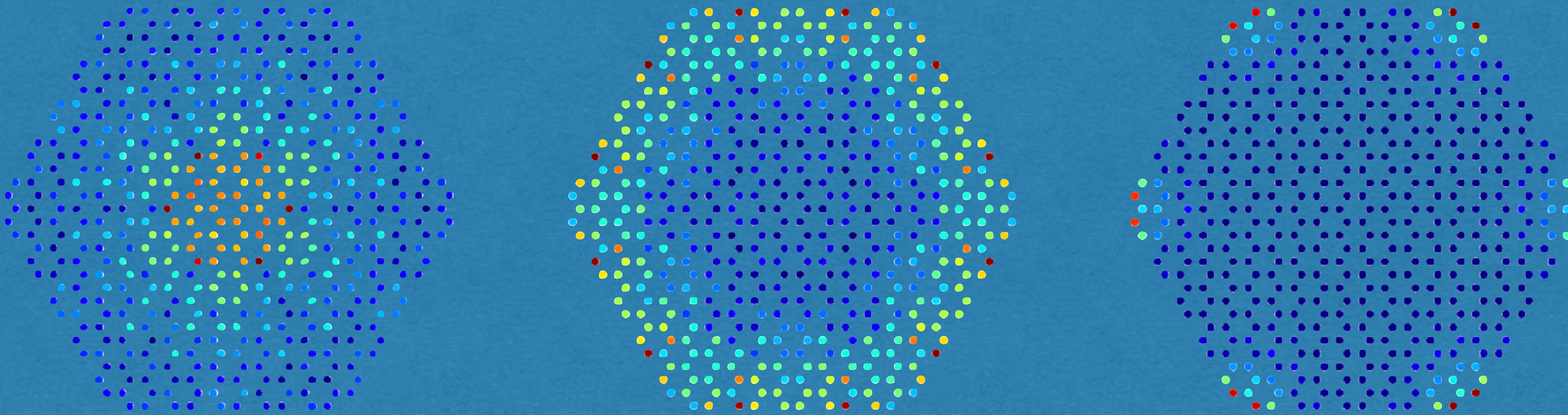

Quantized Boundary Charges in 2D Spin-Orbit Coupled Crystals

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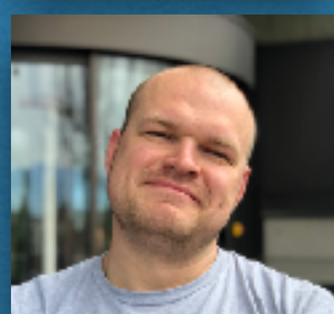
Collaborators



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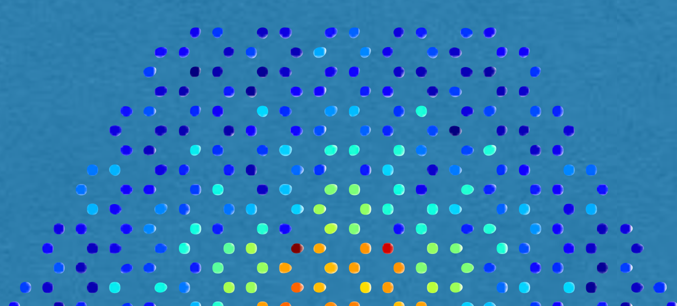
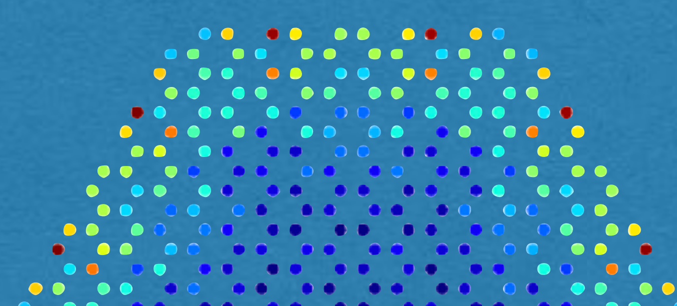
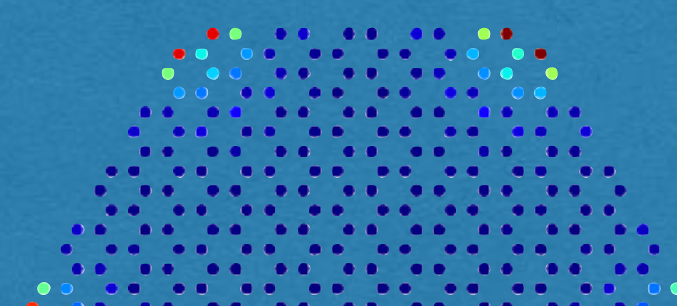
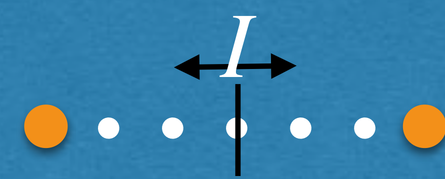
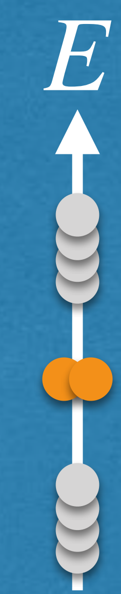




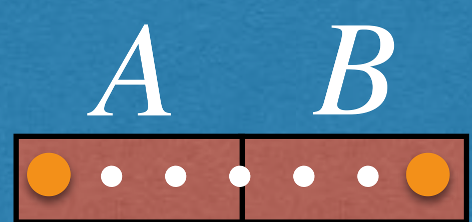
Charge Fractionalization in 1D

Inversion symmetric
Su-Schrieffer-Heeger model



gapped bulk
quantized 1/2 end charges

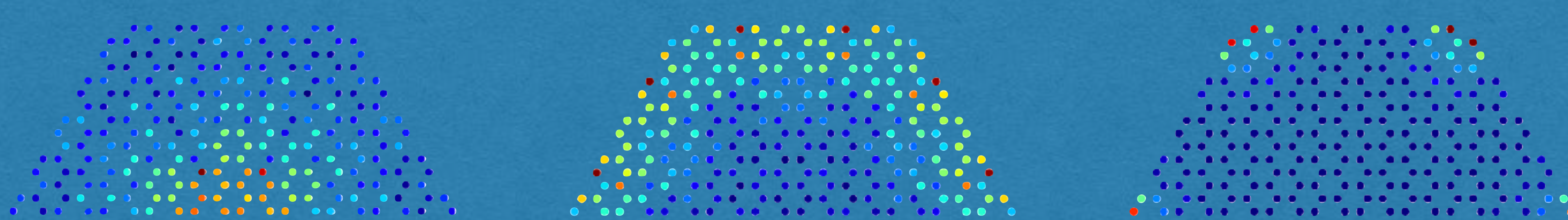




$$Q_A + Q_B \in \mathbb{Z}, \quad Q_A = Q_B$$

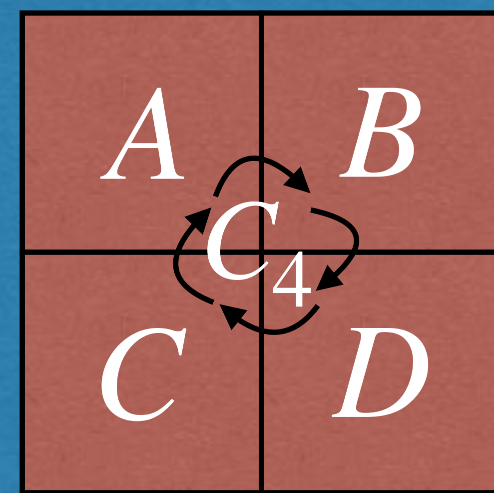
$$Q_A = 0,\ 1/2 \mod 1$$

0D midgap states are not protected by crystal symmetries, but fractional boundary charges are!



Charge Fractionalization in 2D

Four-fold rotationally symmetric obstructed atomic limit phase



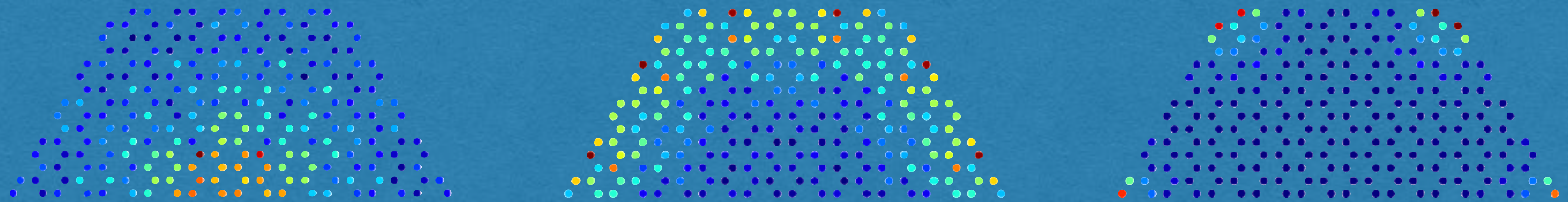
$$Q_A + Q_B + Q_C + Q_D \in \mathbb{Z}, \quad Q_A = Q_B = Q_C = Q_D$$

$$Q_A = 0,\ 1/4,\ 2/4,\ 3/4 \mod 1$$

see also:

Phys. Rev. B 98, 081110(R) by **van Miert** and **Ortix**

arXiv:1809.02142 by **Benalcazar, Li** and **Hughes**



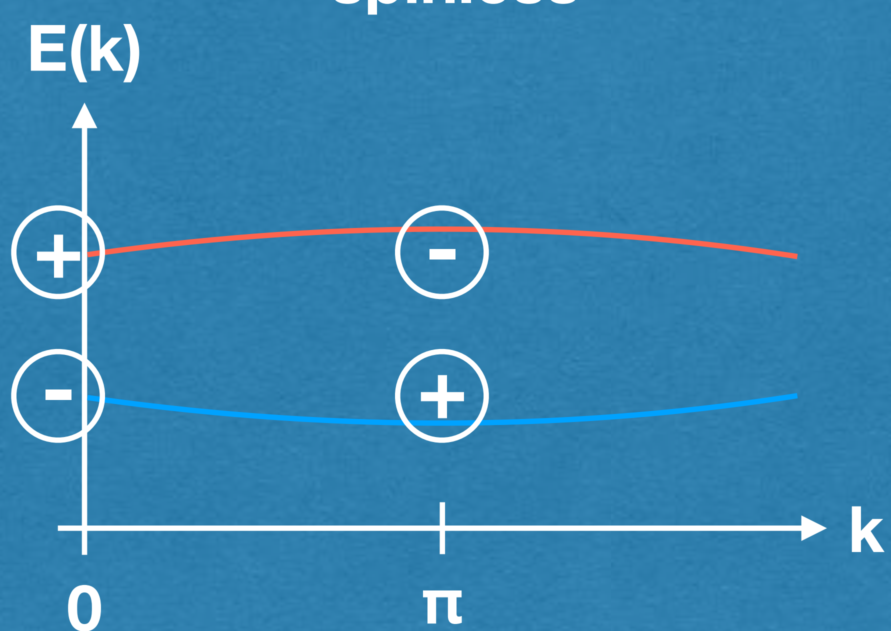
Spinful Time Reversal Symmetry

Introducing spin and time-reversal symmetry has two effects:

1) All charges are doubled: $Q_A \rightarrow 2Q_A$

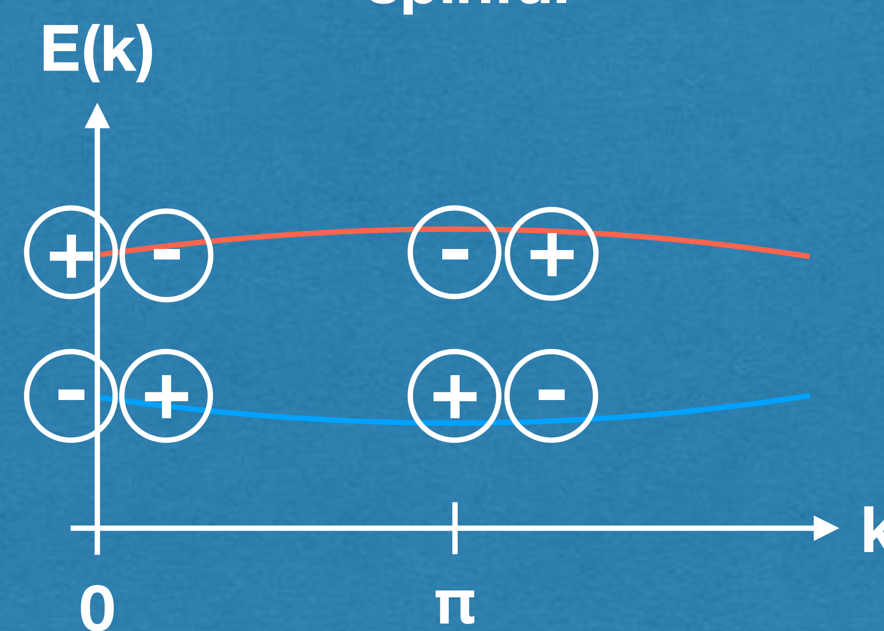
2) We lose some topological invariants:

spinless

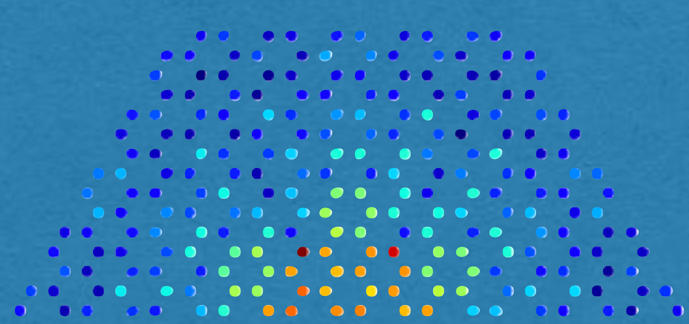


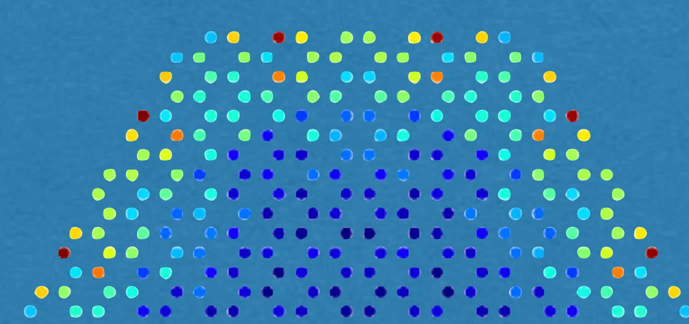
$$(C_2)^2 = 1 \rightarrow C_2 = \pm 1$$

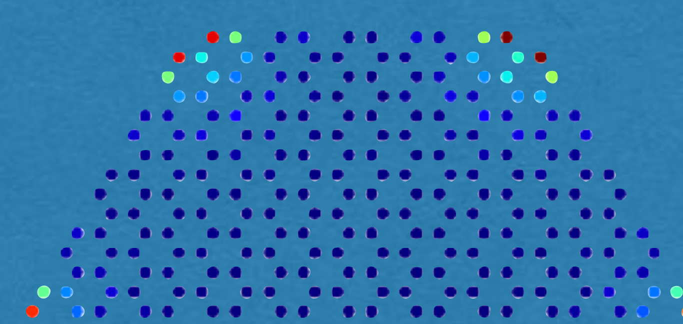
spinful



$$(C_2)^2 = -1 \rightarrow C_2 = \pm \mathrm{i}$$
$$T(+\mathrm{i})T^\dagger = -\mathrm{i}$$



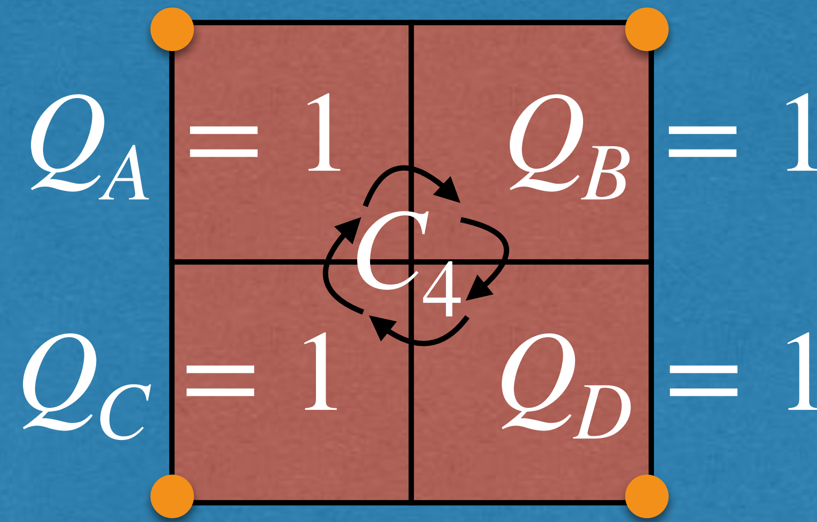




C_4 + TRS insulator in 2D

This phase was introduced in Phys. Rev. Lett. 119, 246402, by Z. Song, Z. Fang, C. Fang

$$H = \left(\textbf{2DTI} \oplus \textbf{2DTI}\right)$$
$$+C_4, T\textbf{-preserving coupling}$$

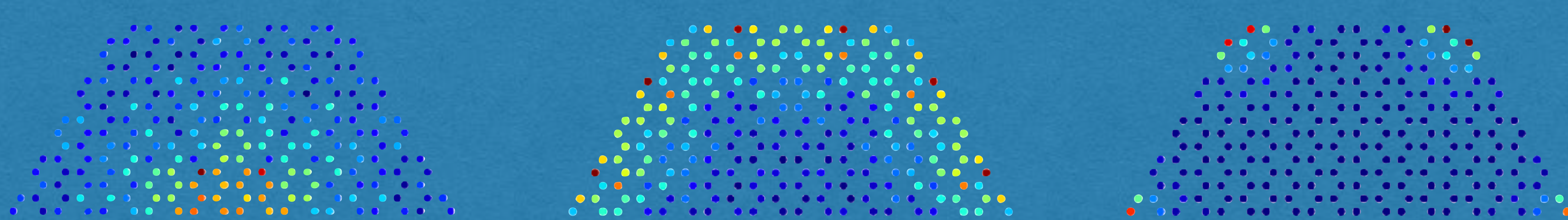


mod 2

The only way to diagnose it so far has been via explicitly determining the maximally localized Wannier centers.

Our invariant: $(C_4)^4 = -1 \rightarrow C_4 = e^{\pm i\frac{\pi}{4}},\ e^{\pm i\frac{3\pi}{4}}$

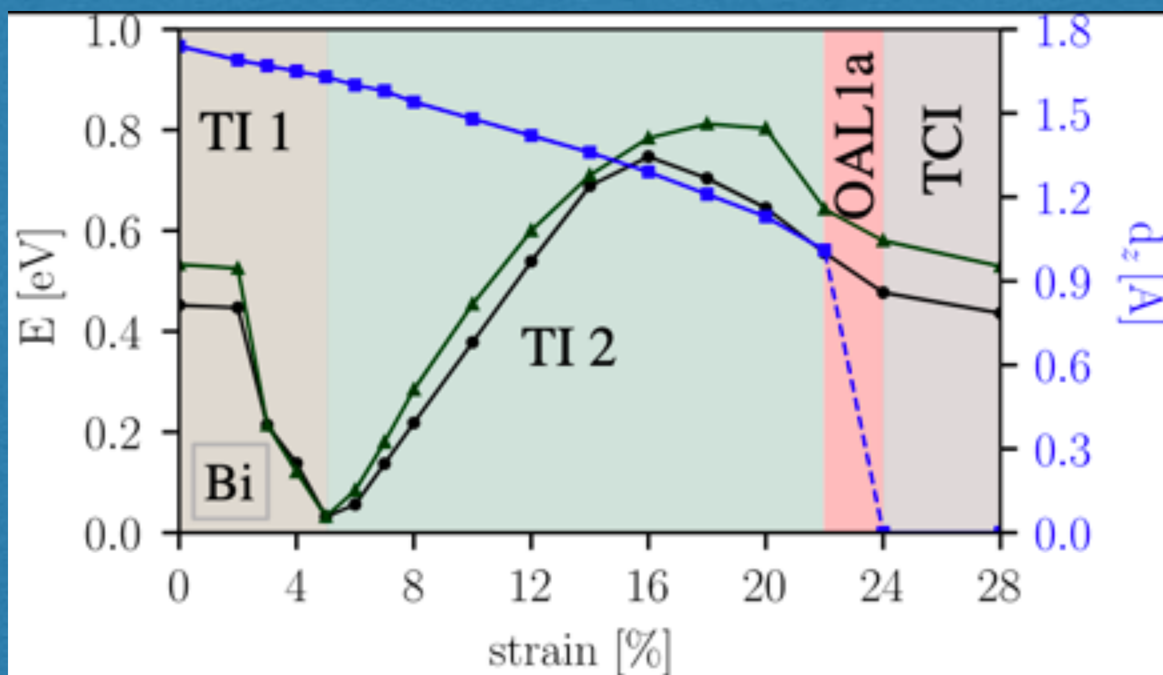
$\rightarrow \mathbb{Z}_2$ **2DTI invariant in both** C_4 **subspaces**

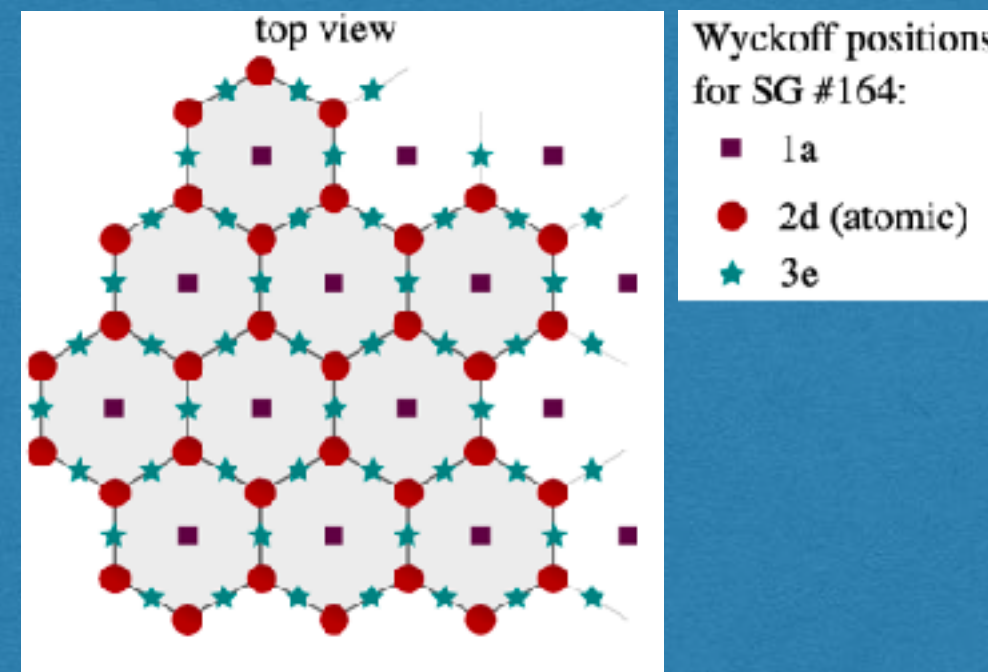


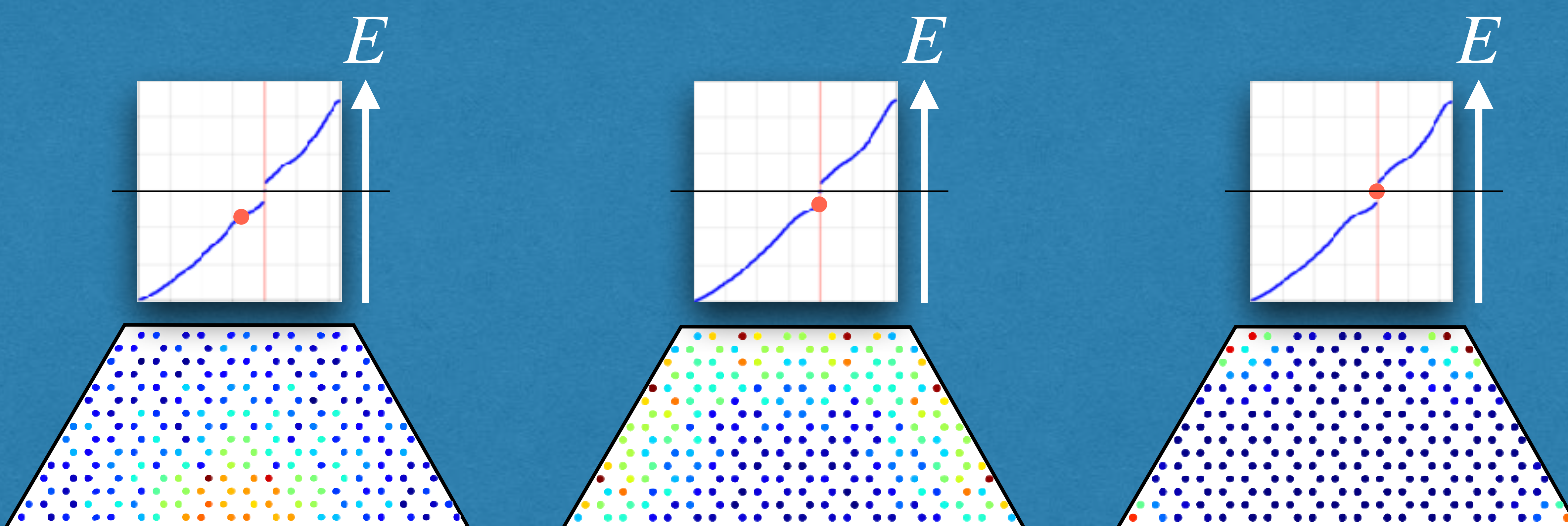
Material Candidates

For the **first time**, we present material candidates for 2D charge fractionalization

Using **DFT**, we calculated the phase diagrams for **Sb**, **Bi**, **As** monolayers
as a function of tensile strain







Summary of Results

For 2D crystals with spatial symmetries and spinful time-reversal, we

1. Prove that fractionalized boundary charges are stable
2. Provide an exhaustive list of topological invariants
3. Map invariants to Wannier centres
4. Map Wannier centres to fractional boundary charges
5. Provide realistic material candidates

Thank you for your attention!