Double Band Inversion in TMD XTe_2

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Overview

1. DBI in TMD
2. Topology in β phase
3. Tight-Binding Model for MNL
4. Topology in γ phase

Why I am interested in DBI

Zhijun Wang (2019)

Higher-Order Topology, Monopole Nodal Lines, and the Origin of Large Fermi Arcs in Transition Metal Dichalcognides XTe_2 (X = Mo,W)

PRL 123,186401 (2019)

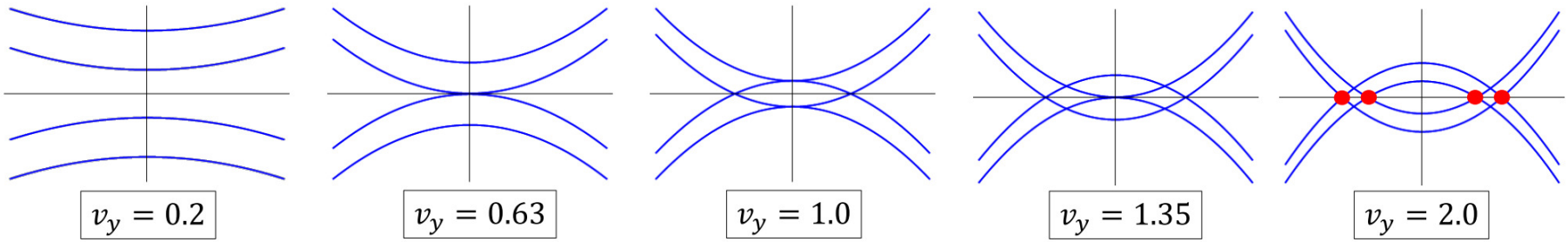


Figure: Bands

TMD Structure

Room temperature: hexagonal α phase ($P6_3/mmc$) and distorted monoclinic β phase ($P2_1/m$). Under 250K: β phase transitions into γ phase ($Pmn2_1$)

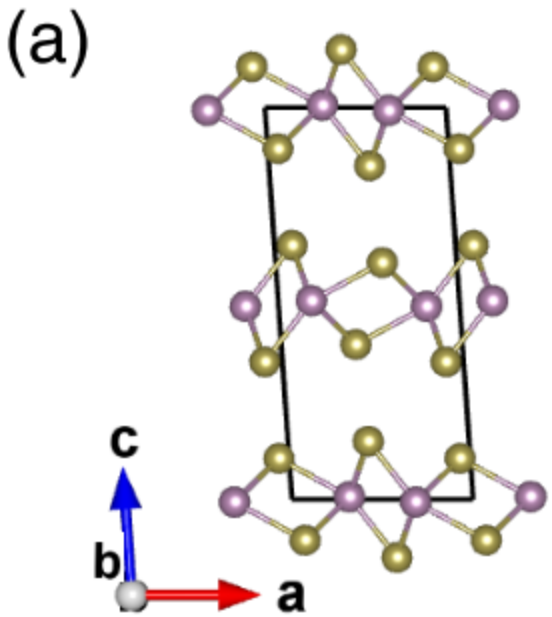
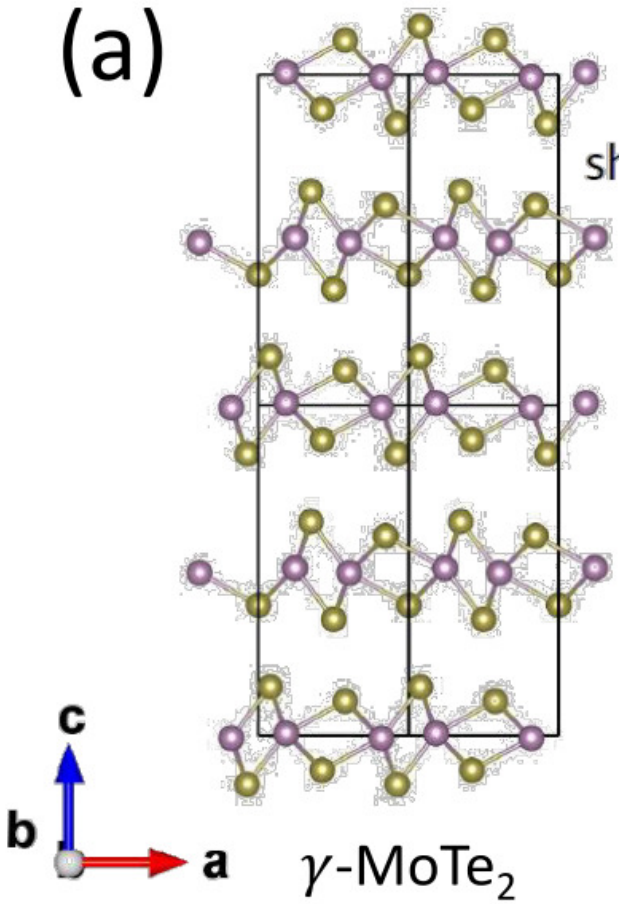


Figure: $\beta-1$T'-$MoTe_2$



γ-$MoTe_2$

DBI in TMD

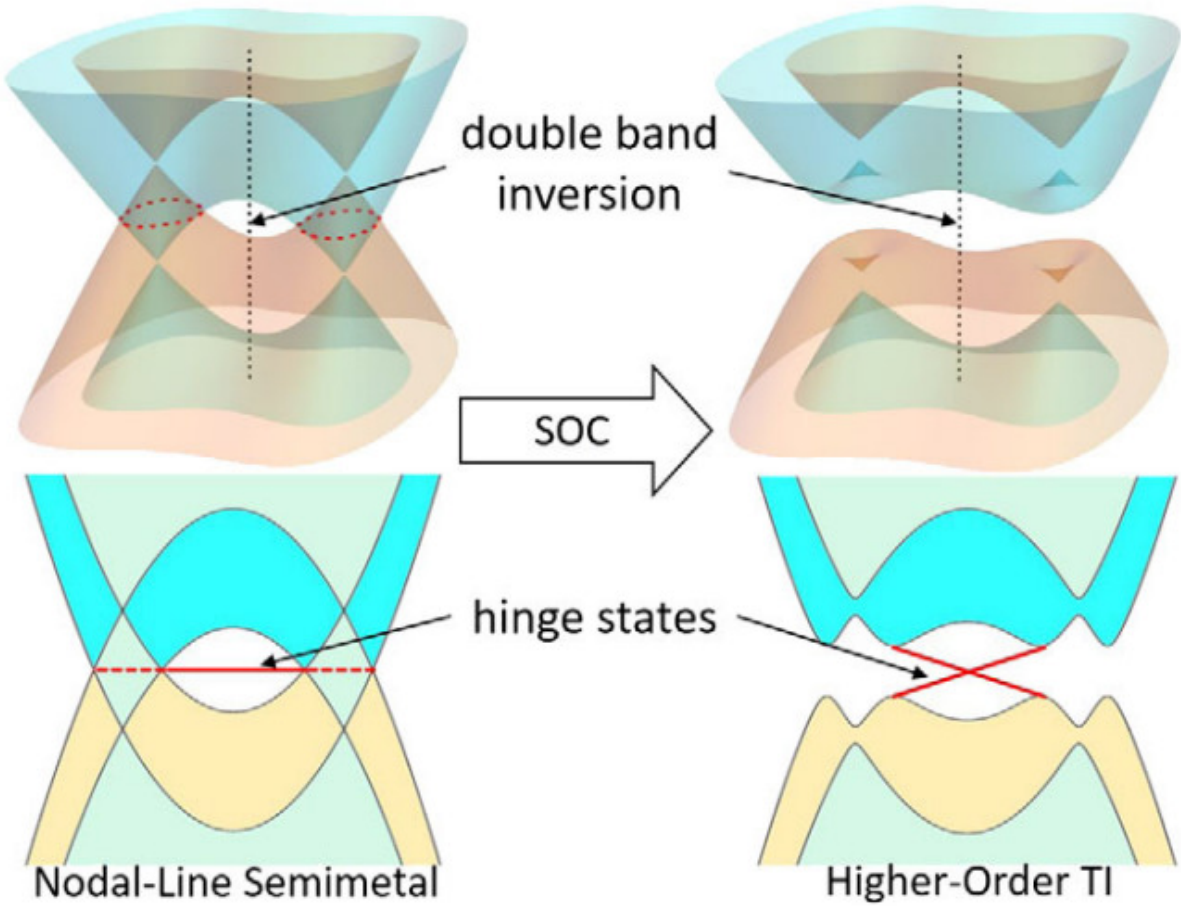


Figure: DBI

Monopole Nodal Line and HOTI in β phase

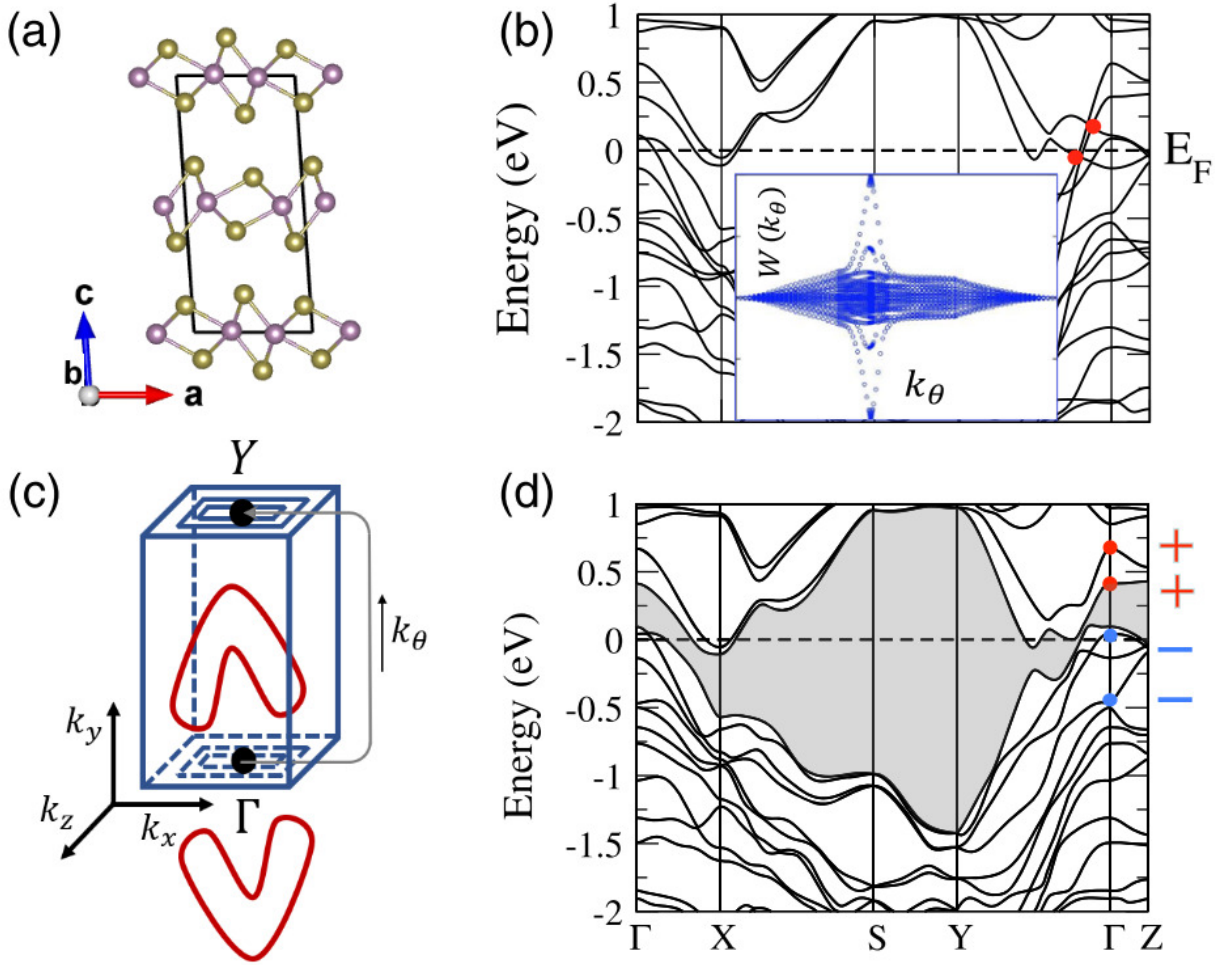
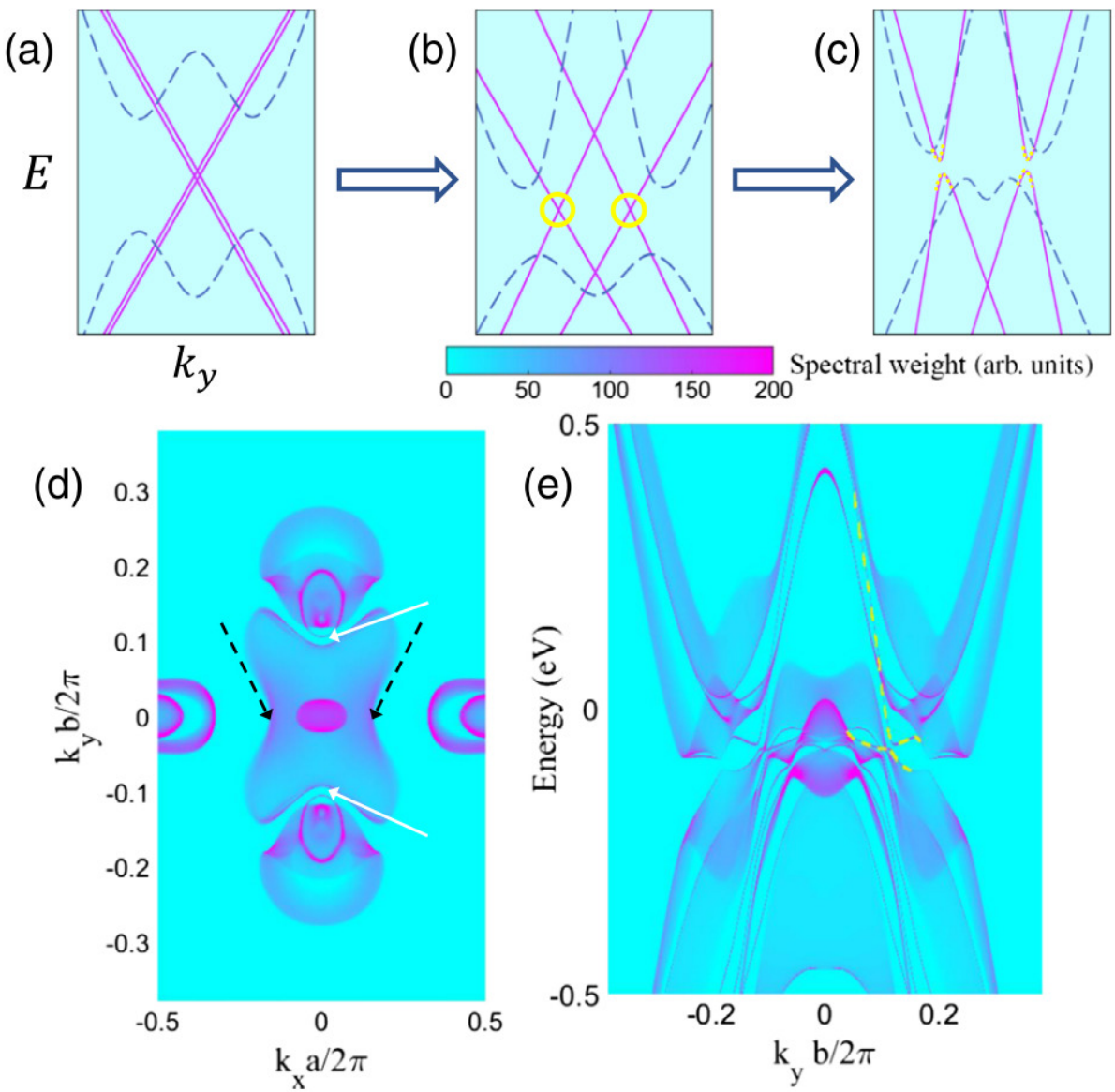


Figure: MNL

TRIM	Γ	X	Y	Z	S	T	U	R
$n_{-}(\vec{k})$	12	14	14	14	14	14	14	14

Figure: The number of Kramers pairs with -1 parity eigenvalues $n_{(k)}$ at each TRIM point in β phase. The Z_2 index can not work anymore. The Z_4 index changed by 2.

surface


(a)
(b)
(c)
E
k_y
0
50
100
150
200
Spectral weight (arb. units)
(d)
(e)
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
k_y b/2π
-0.5
0
0.5
k_x a/2π
0.5
0
-0.5
Energy (eV)
-0.2
0
0.2
k_y b/2π

Tight-Binding Model for MNL

$$H(k) = (m_1 + \sum_{i=x,y,z} v_i cos(k_i))\tau^z + m_2\tau^z\mu^x + m_3\tau^z\mu^z + u_x sin(k_x)\tau^y\mu^y + u_z sin(k_z)\tau^x \quad (1)$$

Orbital τ and μ Pauli matrices.

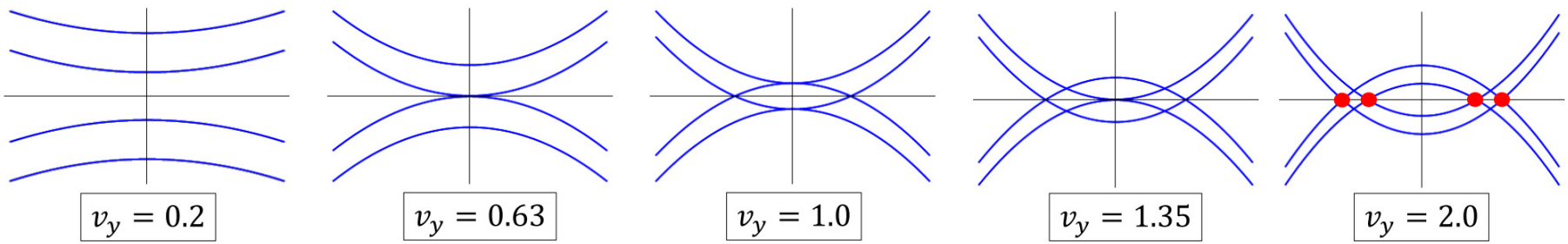


Figure: TB

Under Inversion symmetry and spinless time-reversal symmetry.

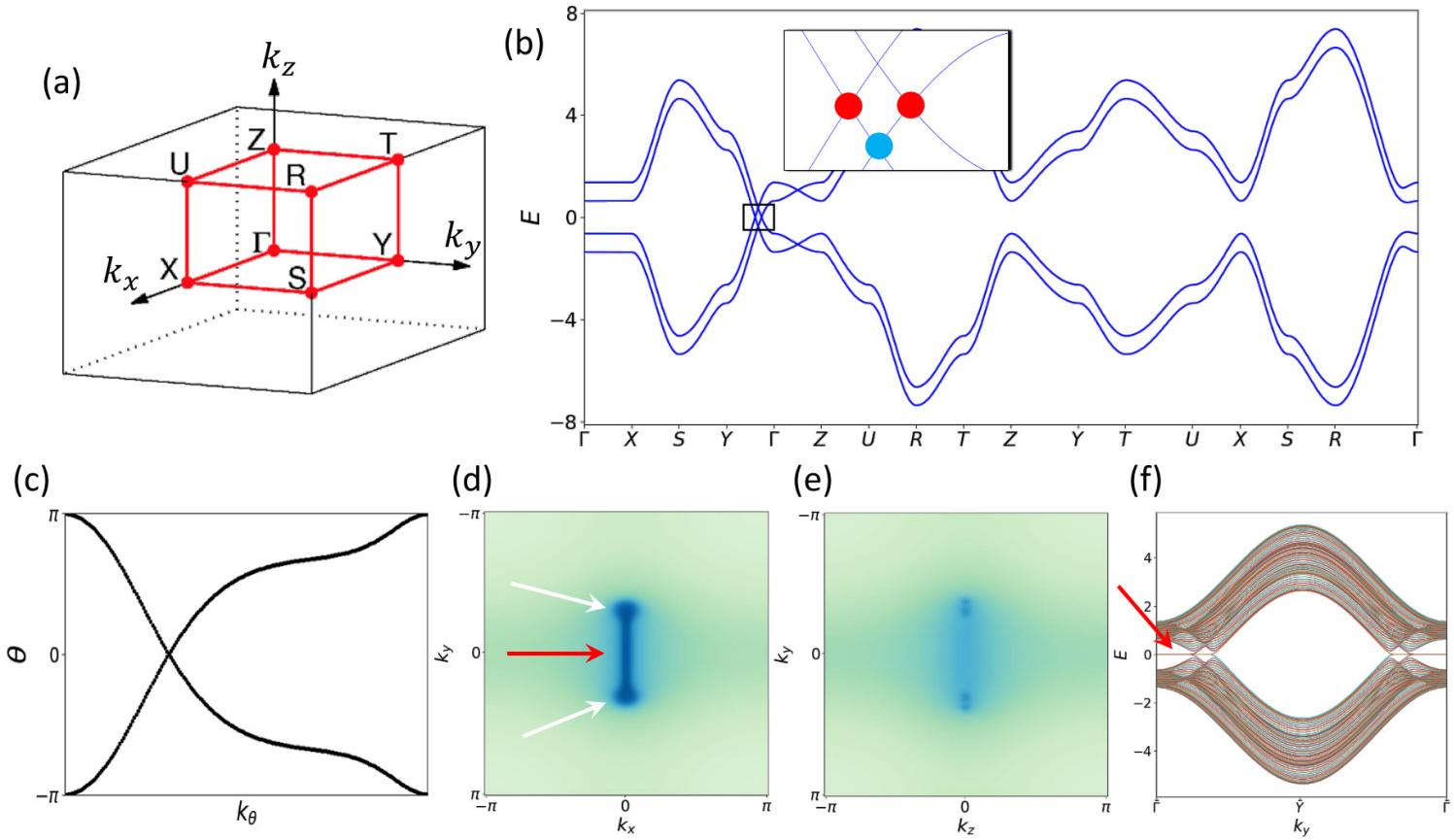

(a)
k_z
Z
T
U
R
Γ
Y
k_y
k_x
X
S
(b)
E
8
4
0
−4
−8
Γ X S Y Γ Z U R T Z Y T U X S R Γ
(c)
θ
π
0
−π
k_θ
(d)
k_y
k_x
(e)
k_y
k_z
(f)
E
4
2
0
−2
−4
Γ Y Γ
k_y

Figure: TB

k.p theory exploit the nested Jackiw-Rebbi construction. Get a term $m_{v1}\mu^z + m_{v2}\mu^x$

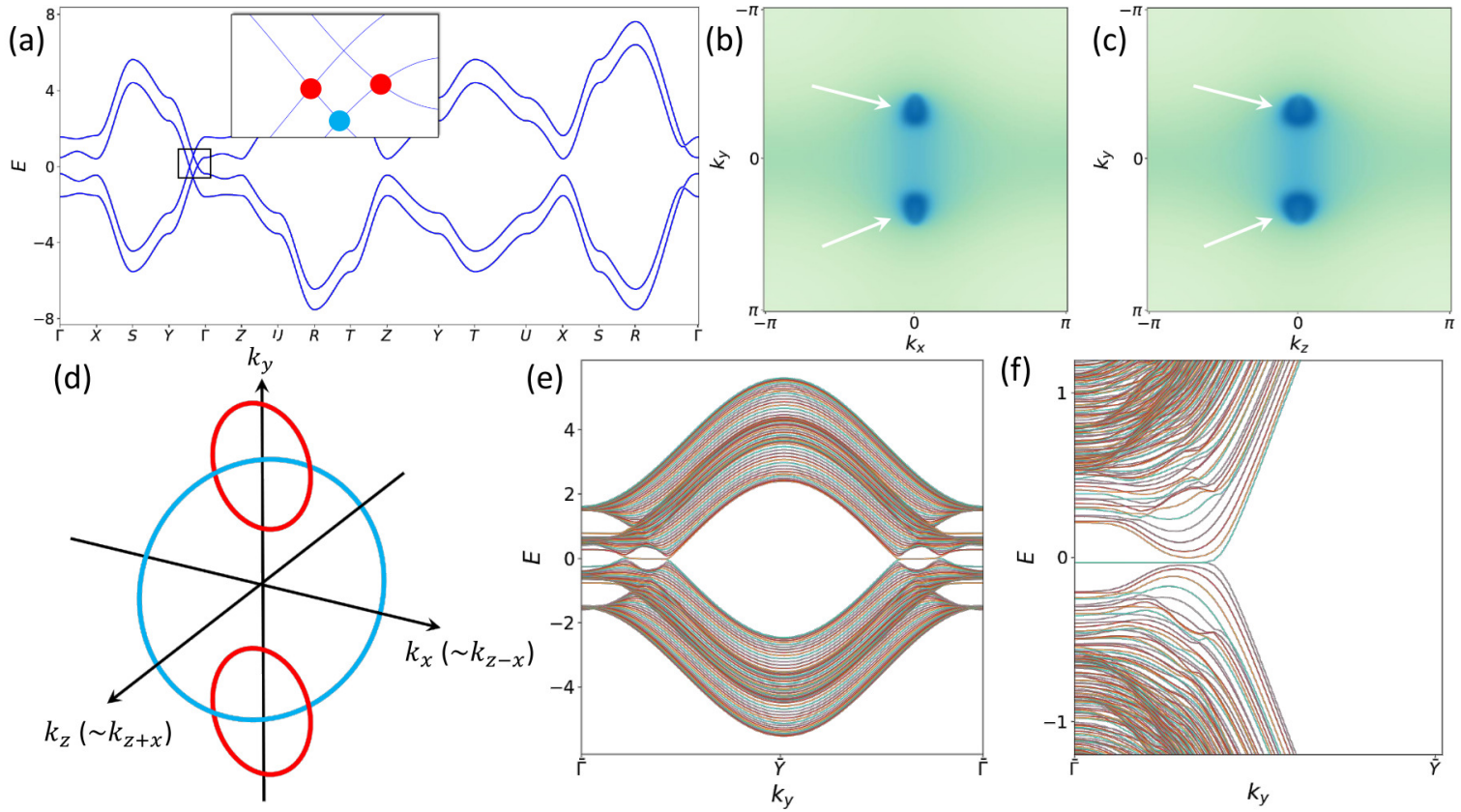


Figure: TB

$$V_{HOIT} = v_H sin(k_y)\tau^y \mu^z \sigma^z$$

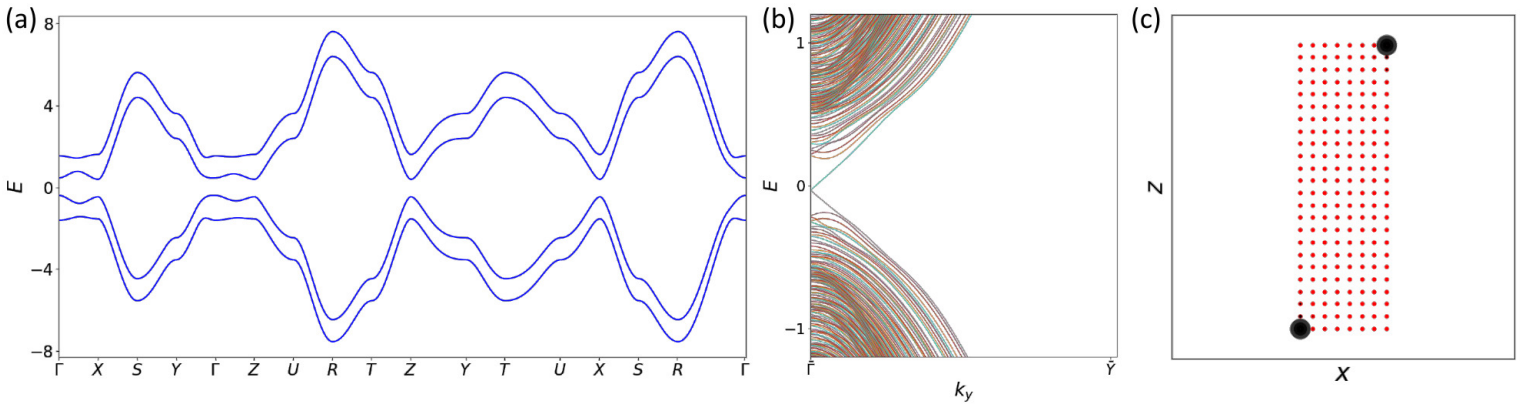


Figure: HOIT

Topology in γ phase

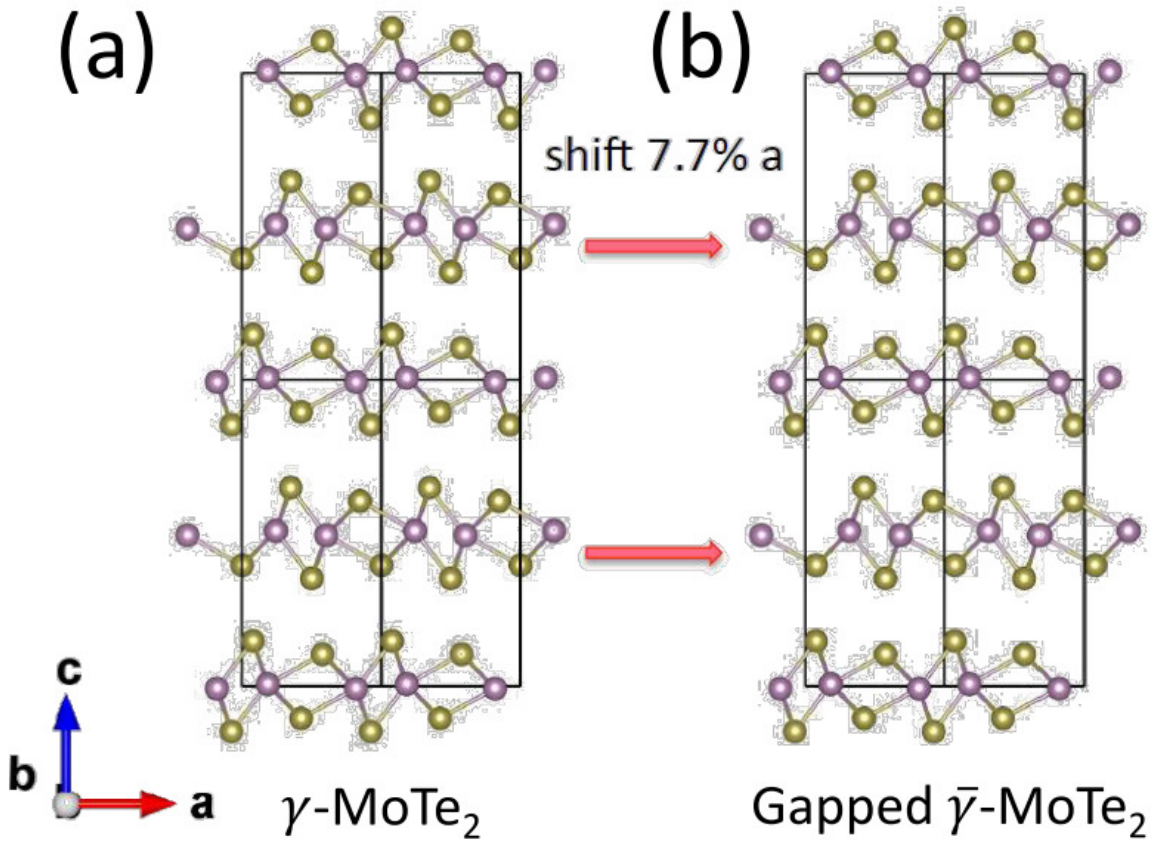


Figure: γ phase

surface

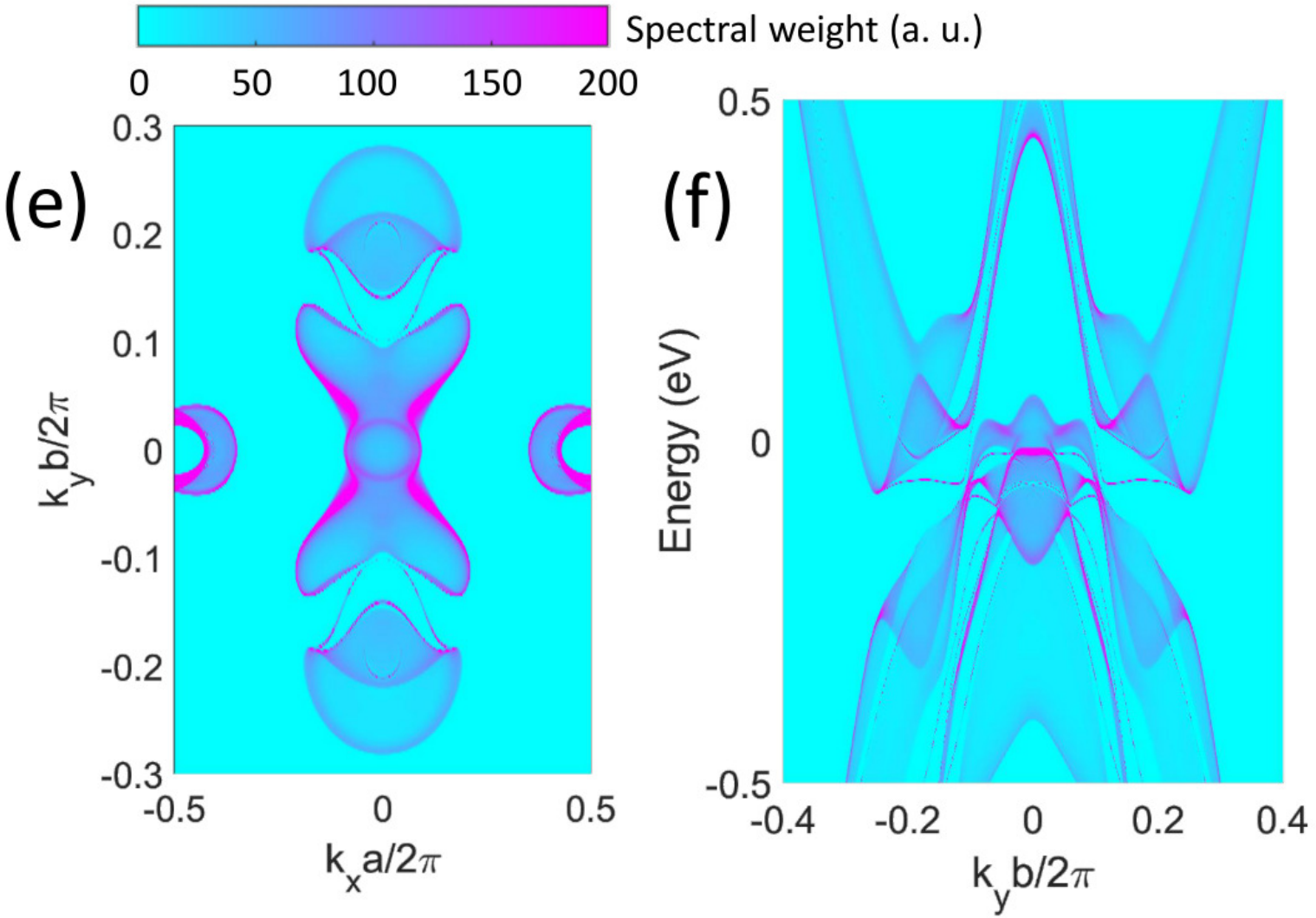


Figure: surface

Origin of Large Fermi arcs

γ-XTe2 crystals also exhibit huge, arclike surface states that largely overwhelm possible signatures of topological Weyl Fermi arcs. Previous works determined these large surface arcs to be topologically trivial. However, in light of our previous analysis of similar nontrivial surface states in β-MoTe2, we recognize this determination to be incomplete. By explicitly calculating the surface states and bulk topology of γ-MoTe2 when its Weyl points are gapped by slight distortion, we, instead, discover that the large Fermi arcs in γ-XTe2 represent the split surface Dirac cones of a nonsymmetry-indicated HOTI phase that is nearby in parameter space and driven by DBI.(A guess)