Antiferromagnetic Topological Insulator $EuSn_2P_2$

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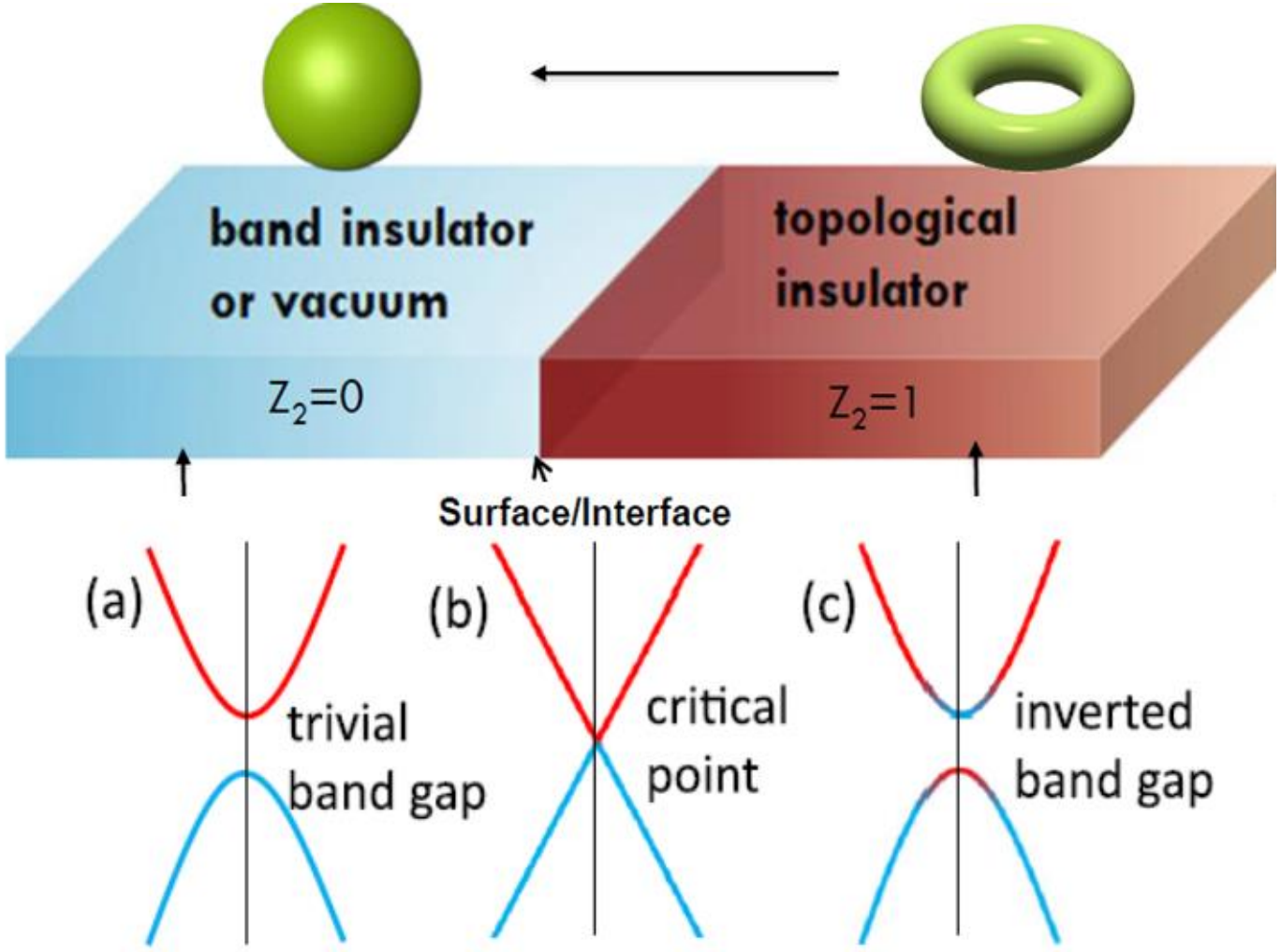
National Cheng Kung University, Department of Physics

Outline

- Progresses on AFM-TI
  Z_2 index in an antiferromagnetic system
  recent results of AFM-TI

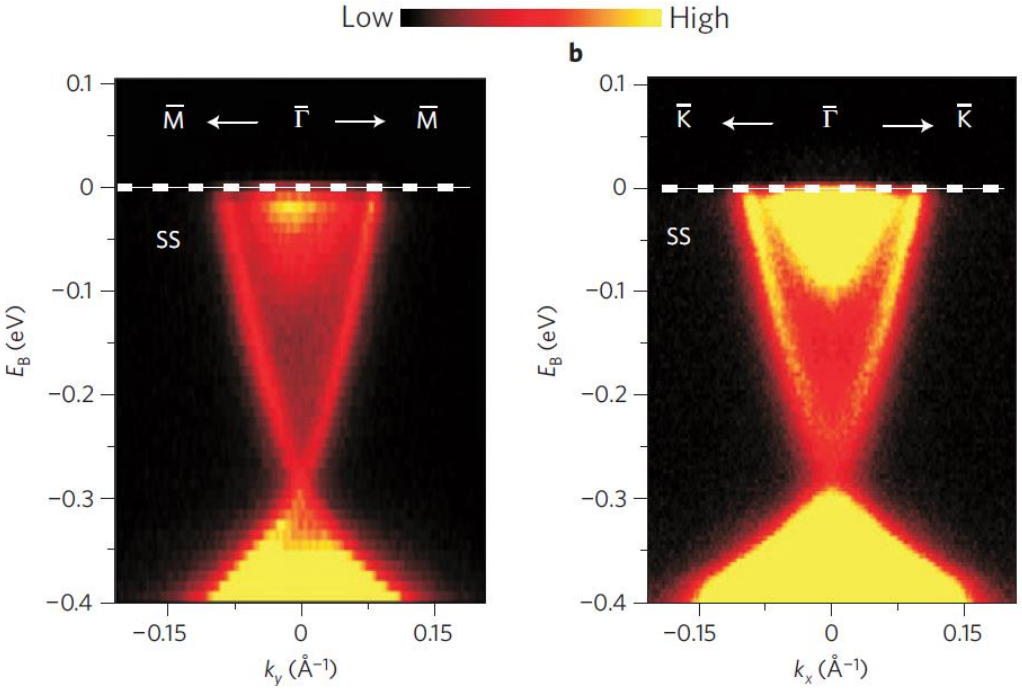
- Calculation results and discussion
  magnetic structure & band structure from DFT
  Z_2 invariant in $EuSn_2P_2$
  Topological Surface states

TI-what's different



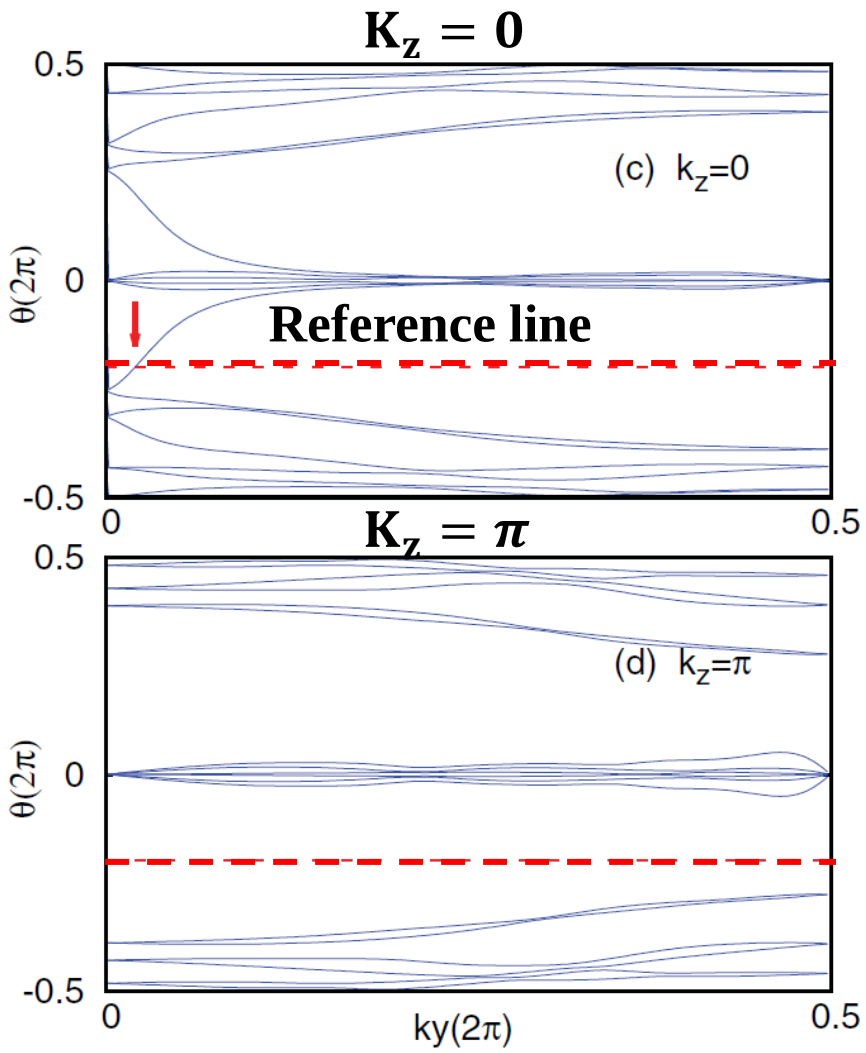
A. Bansil et al. Rev. Mod. Phy. **88** 021004 (2016)

gapless surface states
(protected by Time reversal symmetry)

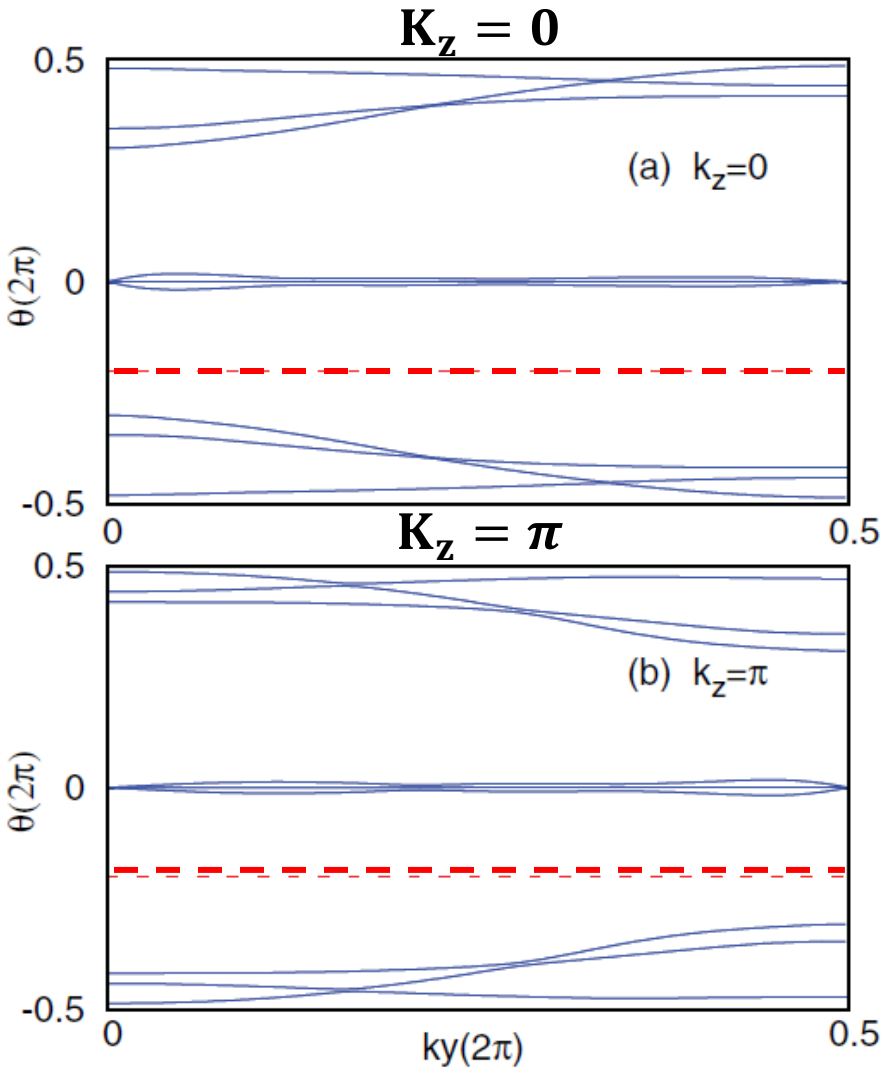


Y. Xia et al. Nature Physics **5**, 398 (2009)

Topological invariant Z_2



Wilson loop of Bi_2Se_3



Wilson loop of $CdTe$

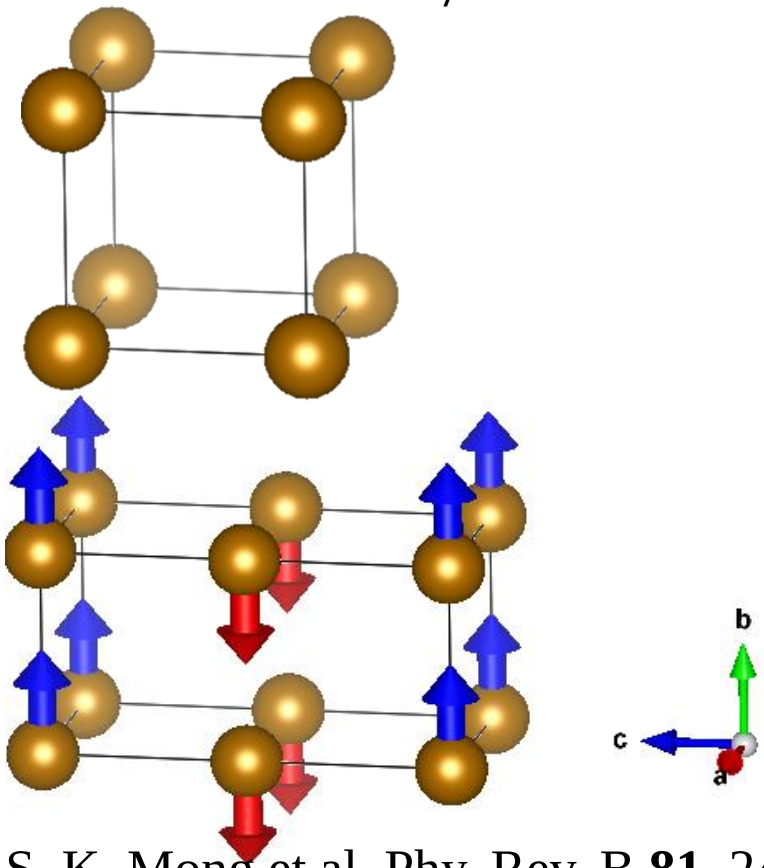
R. Yu et al. Phy. Rev B **84**, 075119 (2011)

Topological invariant in antiferromagnetic topological insulator(AFM-TI)

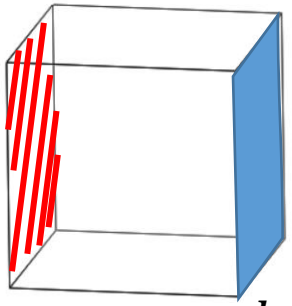
- TRS TI: Z_2 (TRS: time reversal symmetry)
- How about the TRS-breaking system?

  ⇒ a new Z_2 index (if the symmetry $S = \Theta T_{1/2}$ is preserved)

Θ: Time reversal, $T_{1/2}$: primitive translation



$K_z = 0$ $K_z = \pi$



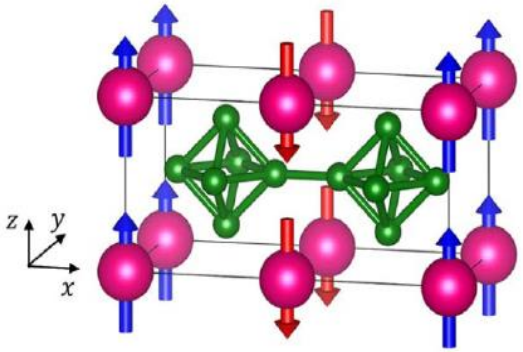
$K_z = 0 \& K_z = \pi$ *are mapping onto the* $K_z^d = 0$

$\gamma_0^d = \gamma_0 + \gamma_\pi = Z_2$

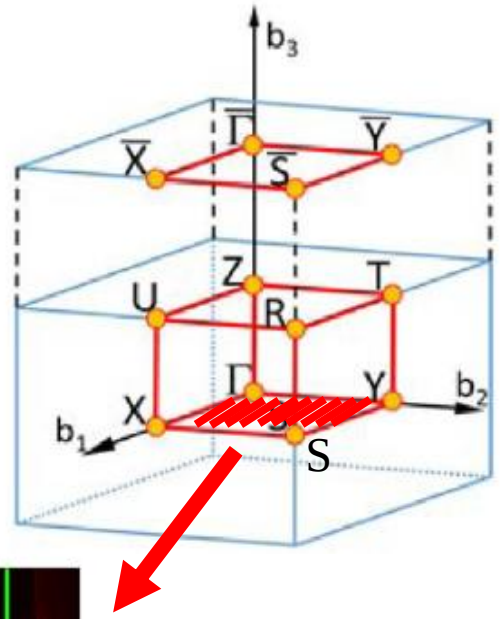
$K_z^d = 0$ $K_z^d = \pi$

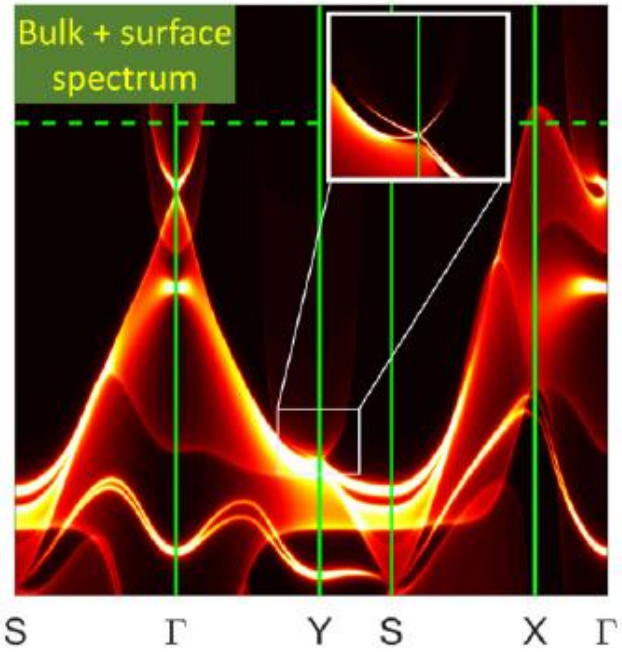
R. S. K. Mong et al. Phy. Rev. B **81**, 245209 (2010)

Progress on AFM-TI



AFM unit cell of SmB6





SmB_6, A-AFM surface states (under pressure 8GPa)

K.W. Chang et al .Phy Rev B **97**, 195145 (2018)

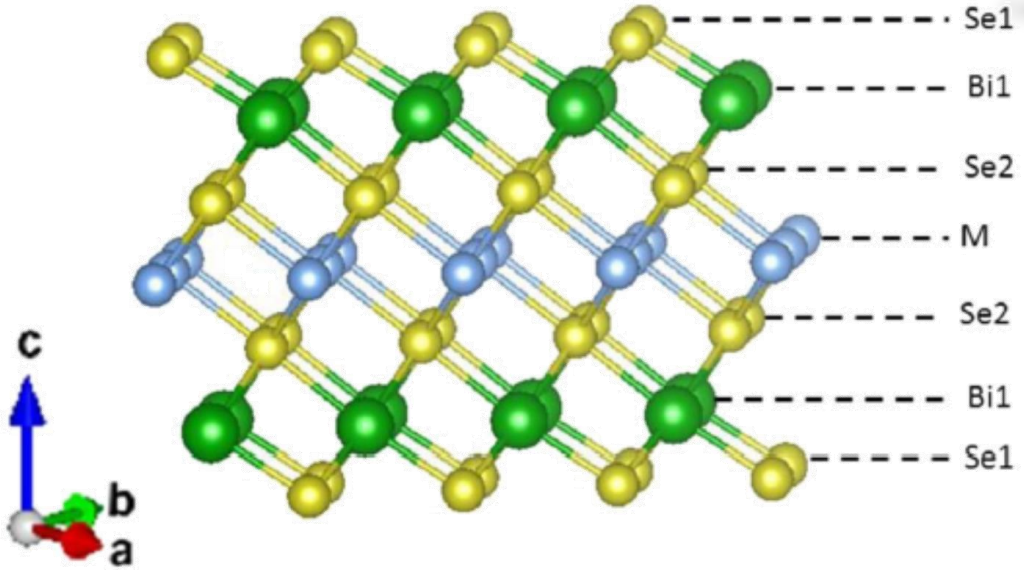


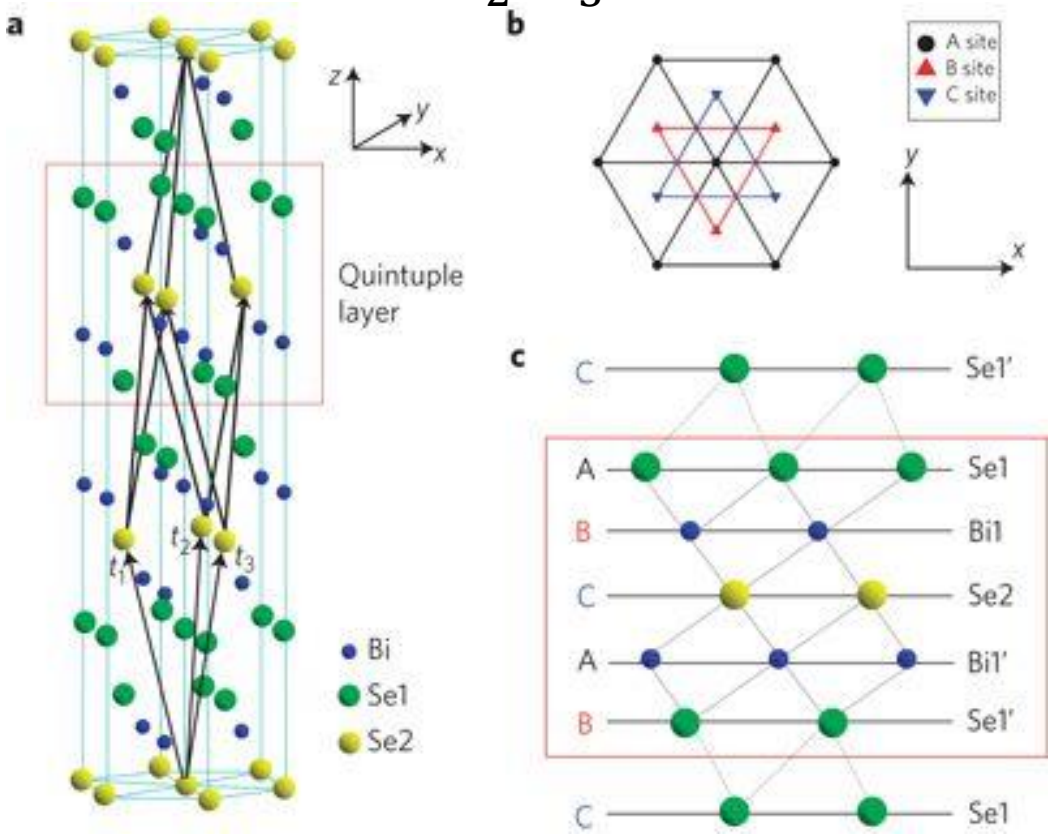
Table 1. Table summarizing the various magnetic orderings and layer thicknesses we consider in this work that have non-trivial topology

Spin ordering	Spin direction	Thickness	Topological phase
AFM	(001)	Bulk	AFM-TI
FM	(001)	Bulk	Weyl semimetal
FM	(100)	Bulk	Weyl line node
AFM (001) surface	(001)	≥7, odd number	Chern insulator
FM (001) surface	(001)	≥3	Chern insulator

S. Chowdhury et al. npj Computational Materials **5**,33 (2019)

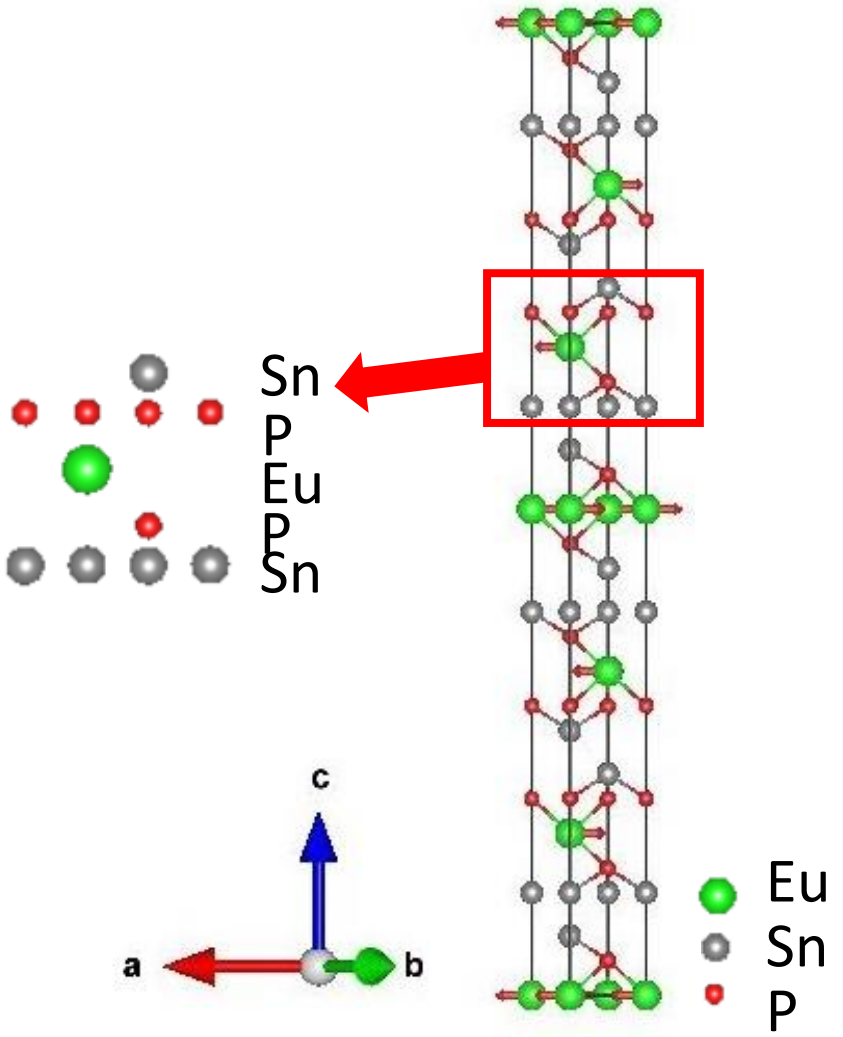
A totally new quantum material-$EuSn_2P_2$

Bi_2Se_3



H. Zhang et al .Nature Physics **5**, 438–442 (2009)

$EuSn_2P_2$



X. Gui et al. ACS Cent. Sci. 2019, **5**, 900−910

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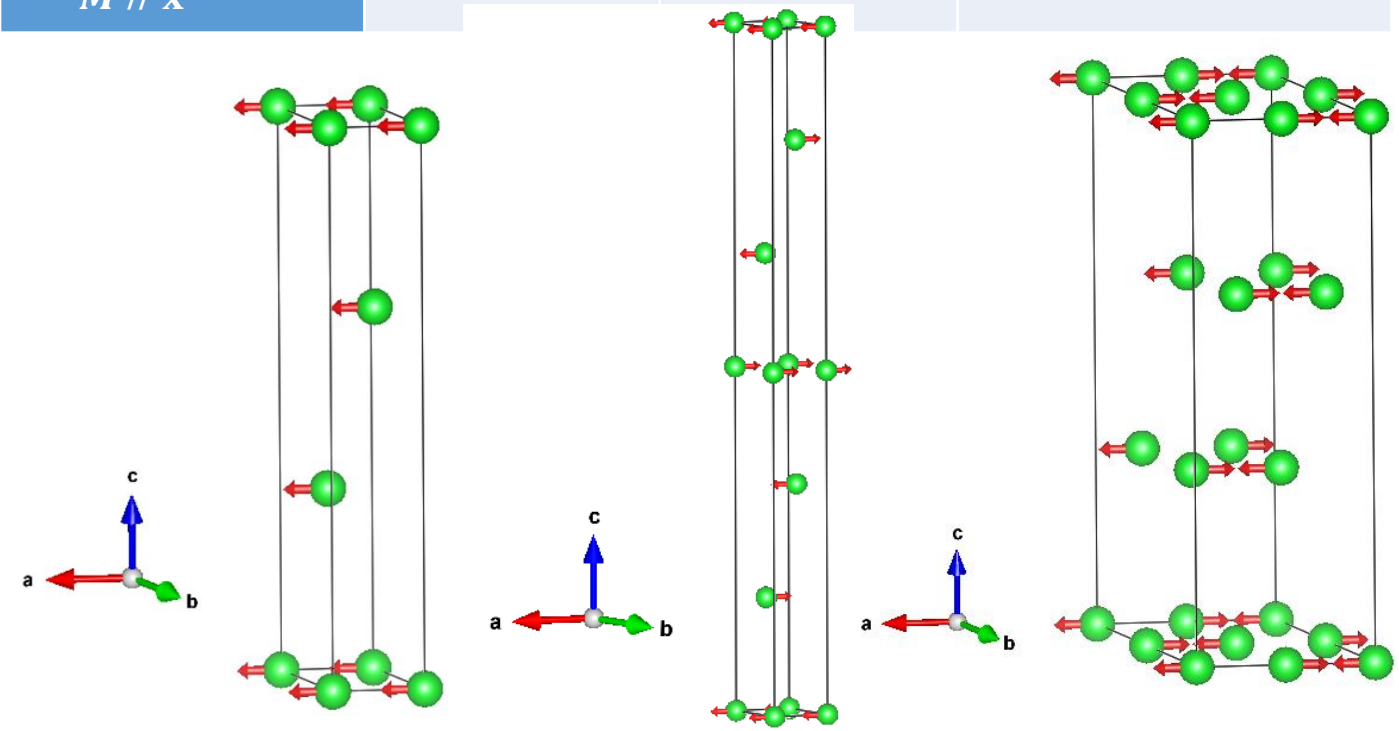
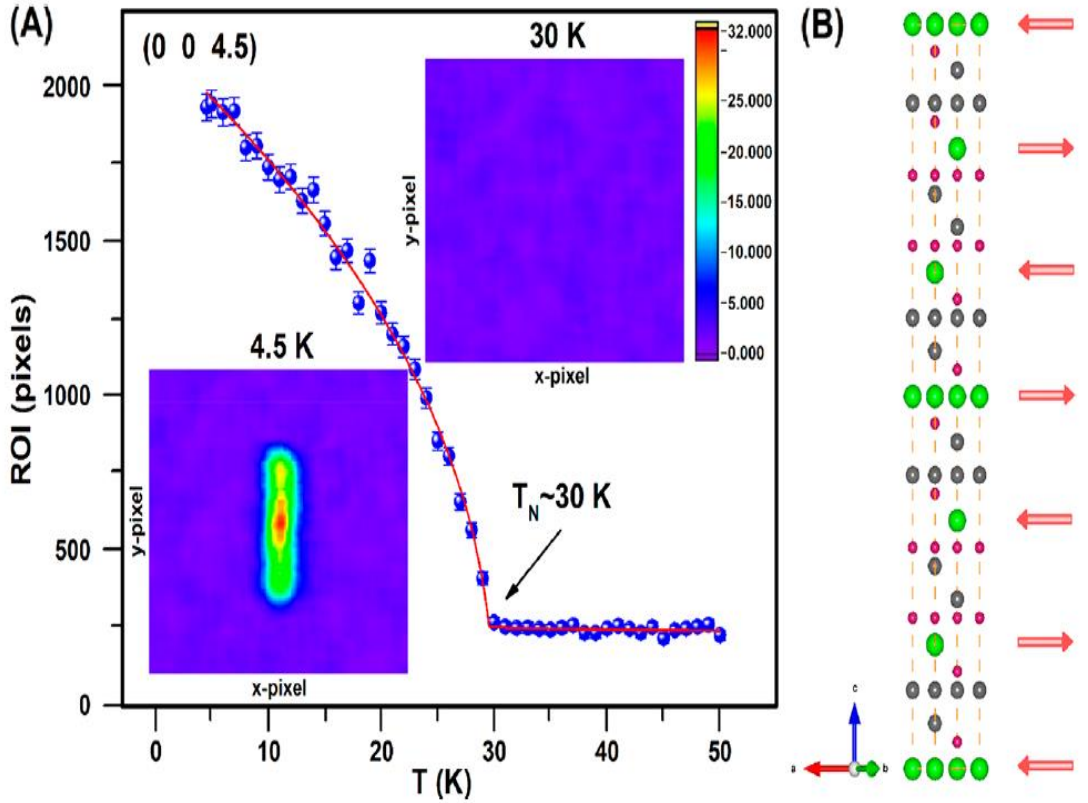
  Topological Surface states

Magnetic structure

Table I. Calculation results of energy of different magnetic structures

	FM	AFM	AFM*
Energy (f.u.) $\vec{M}$ // z	-31.6500V	-31.6536eV	-31.6441eV
Energy (f.u.) $\vec{M}$ // x	-31.6521eV	-31.6651eV	-31.6439eV

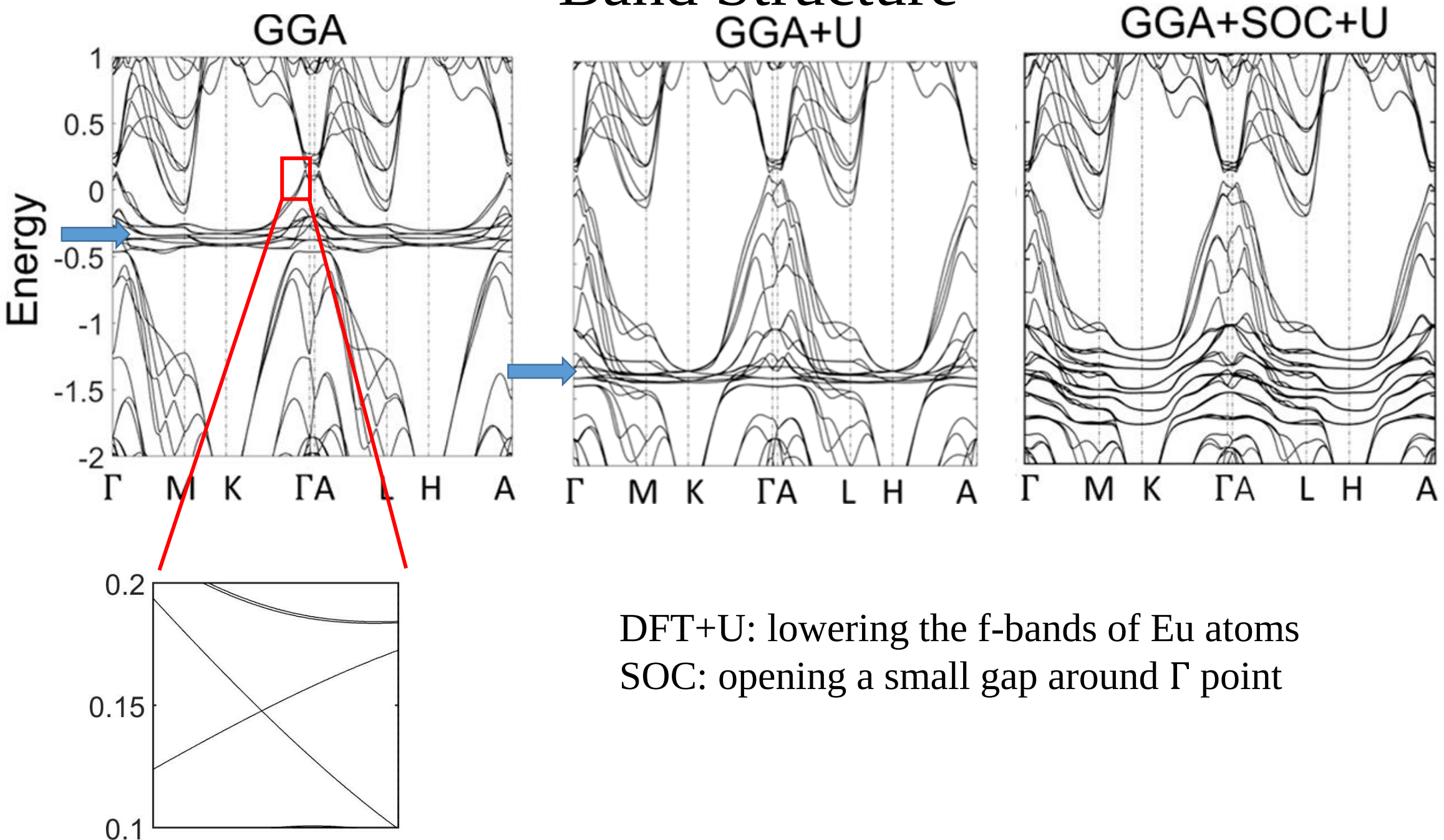




Experimental results show that the magnetic moments lie in the x-direction, which is consistent with the results from DFT.

X. Gui et al. ACS Cent. Sci. 2019, **5**, 900−910

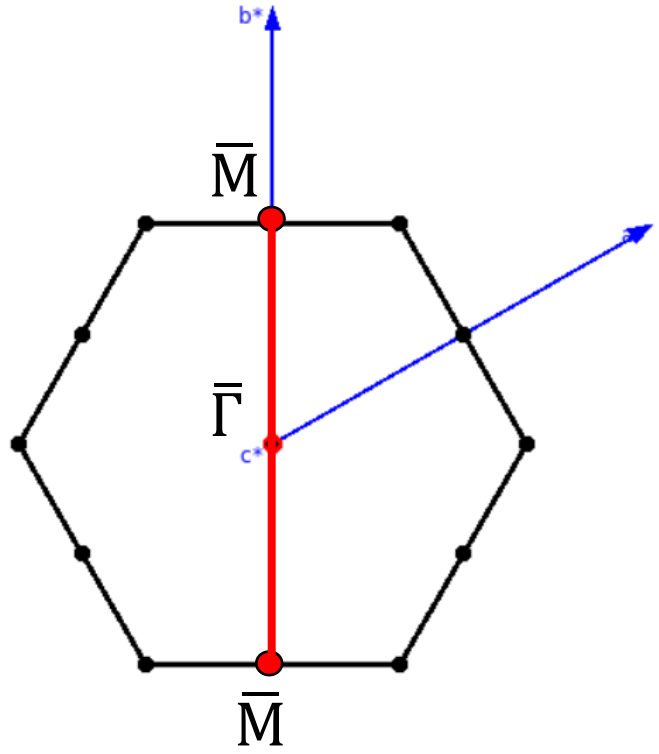
Band Structure



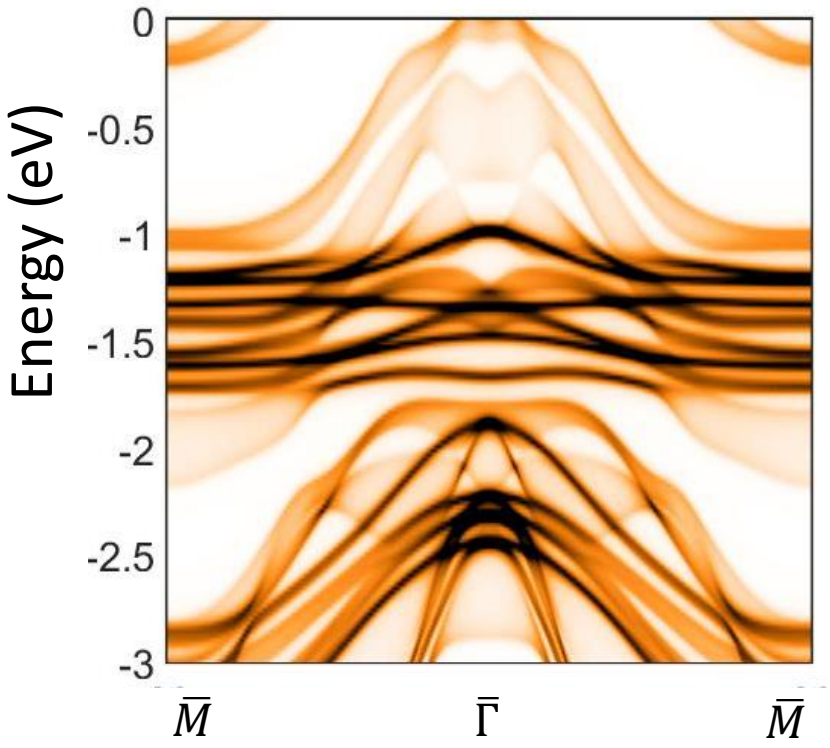
DFT+U: lowering the f-bands of Eu atoms

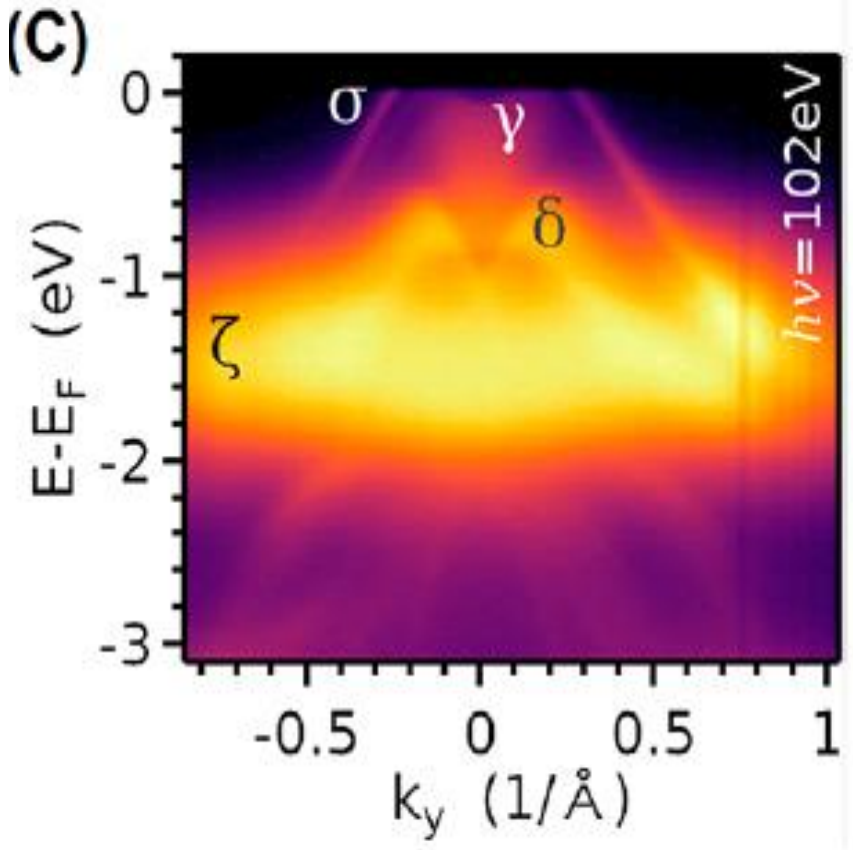
SOC: opening a small gap around Γ point

Experimental ARPES data



Projected (001) SBZ





We have employed the DFT+U formalism so that the f-electrons of the Eu atoms are matched with the ARPES experiment. Here U=4.0eV.

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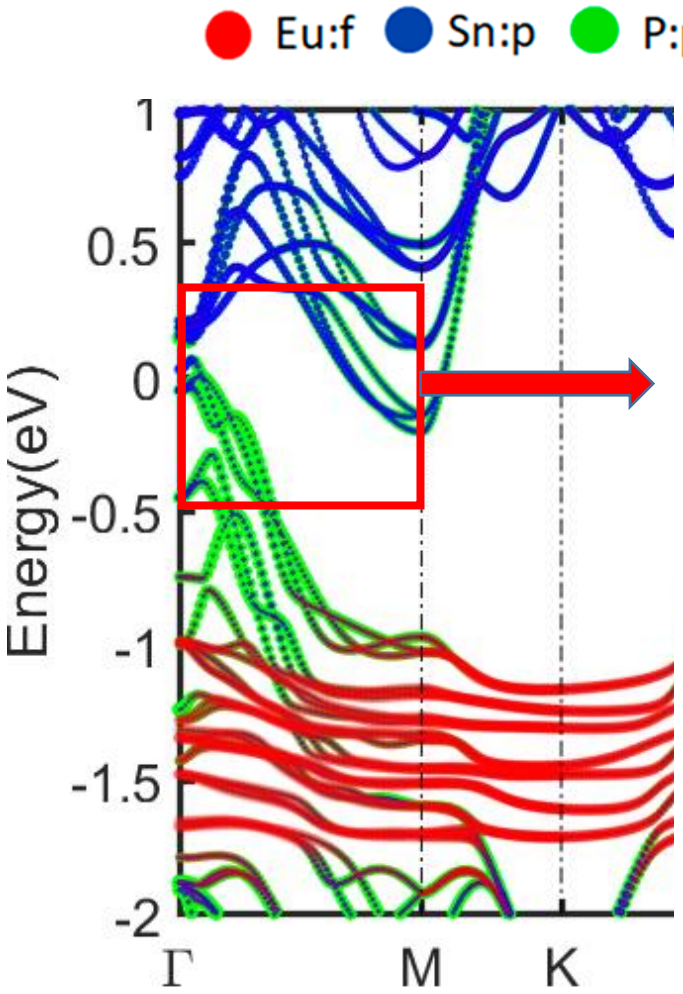
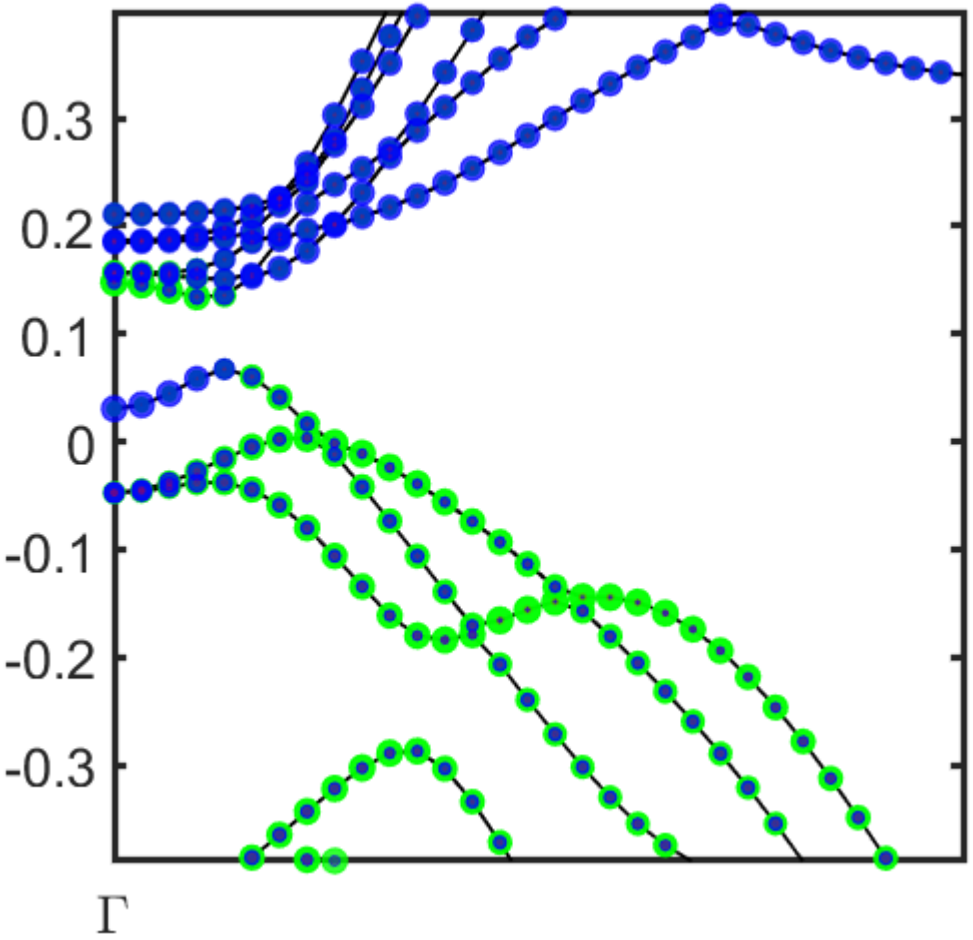
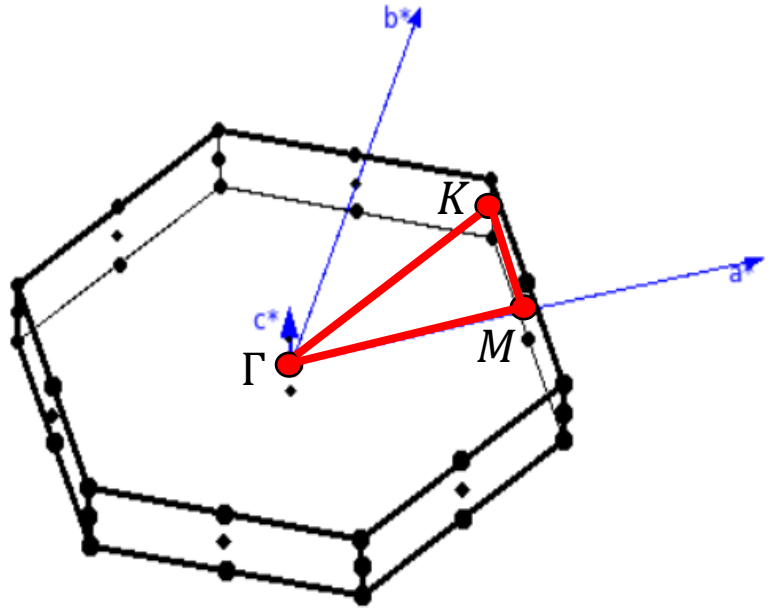
Band Inversion in $EuSn_2P_2$







We observe the band inversion near the Γ point, which is a classical feature of TI.

Topological invariant

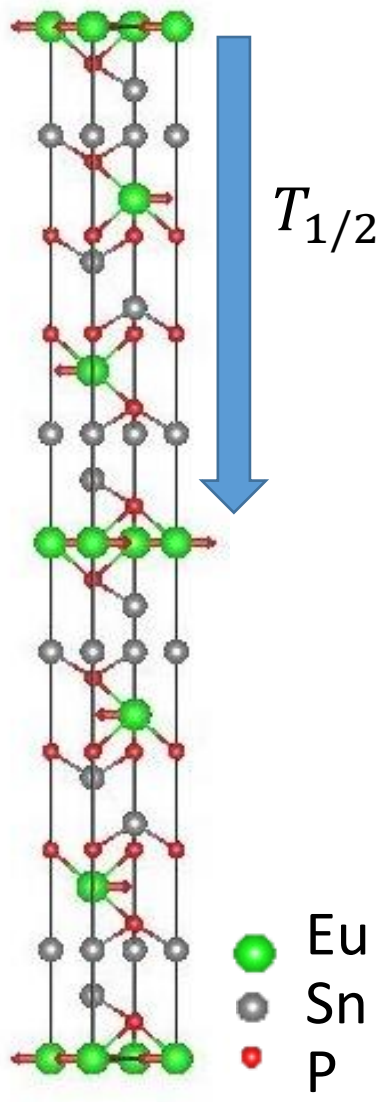
$S = \Theta T_{1/2}$

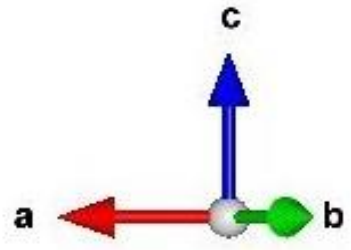
Θ: *Time reversal,*

$T_{1/2}$: *primitive translation*

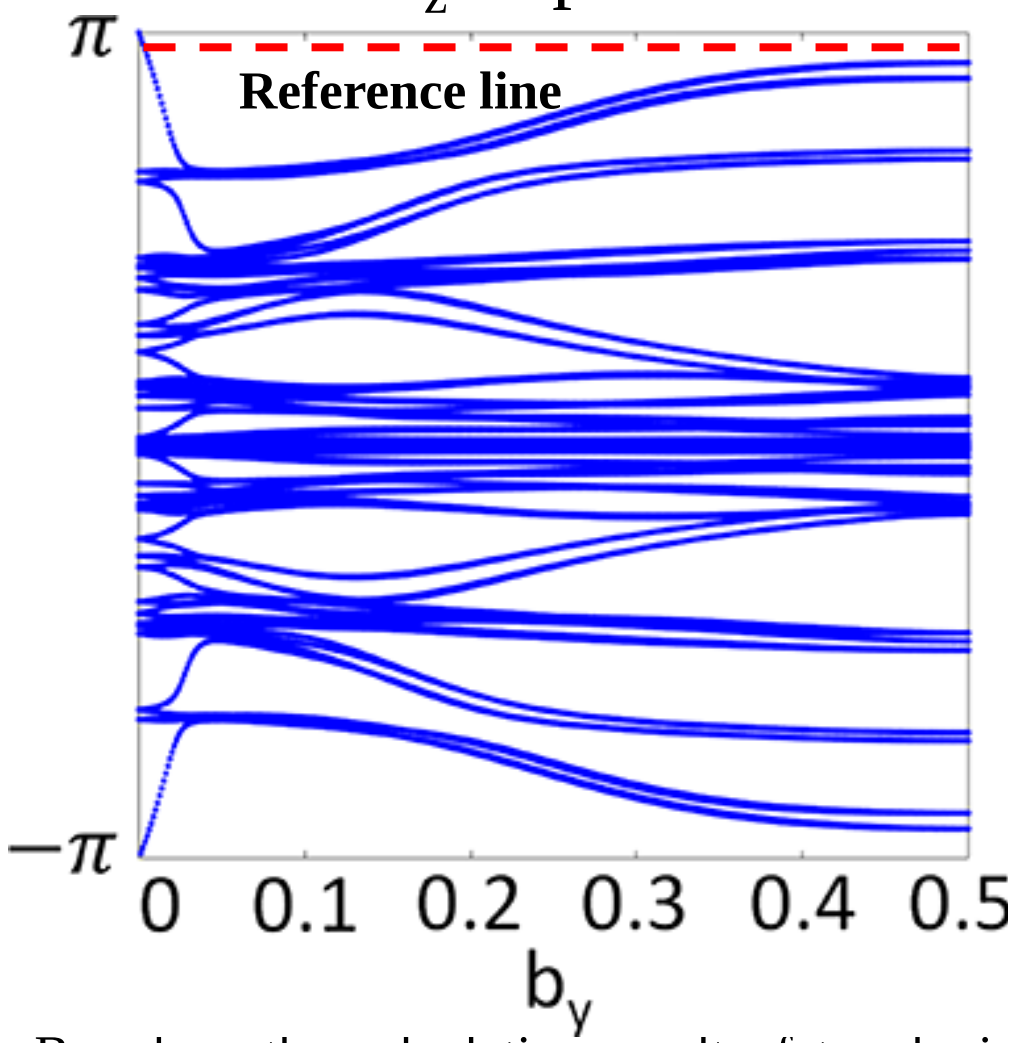
$\hat{T}_{1/2}: \hat{z}$

$EuSn_2P_2$



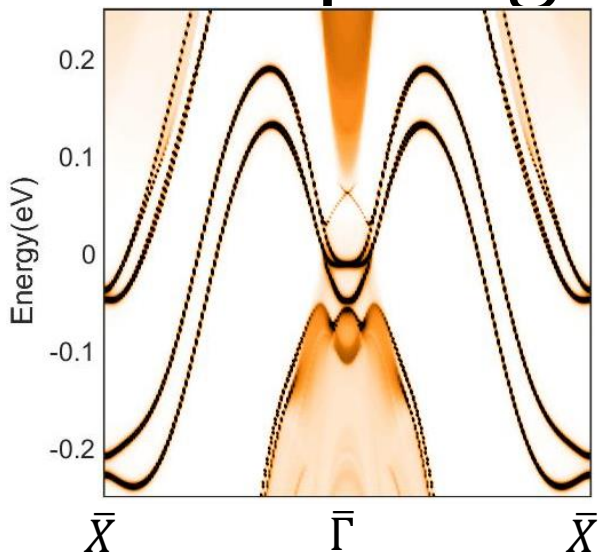


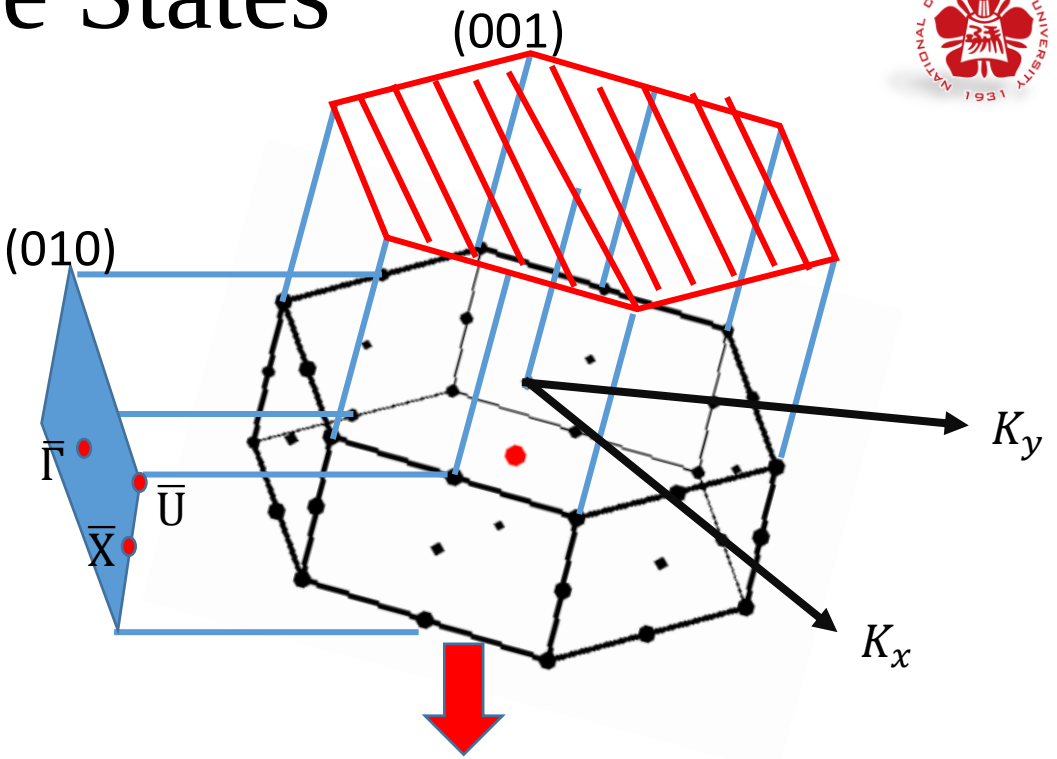
K_z=0 plane



Based on the calculation result of topological invariant Z2, we have identified that the $EuSn_2P_2$ is a antiferromagnetic topological insulator.

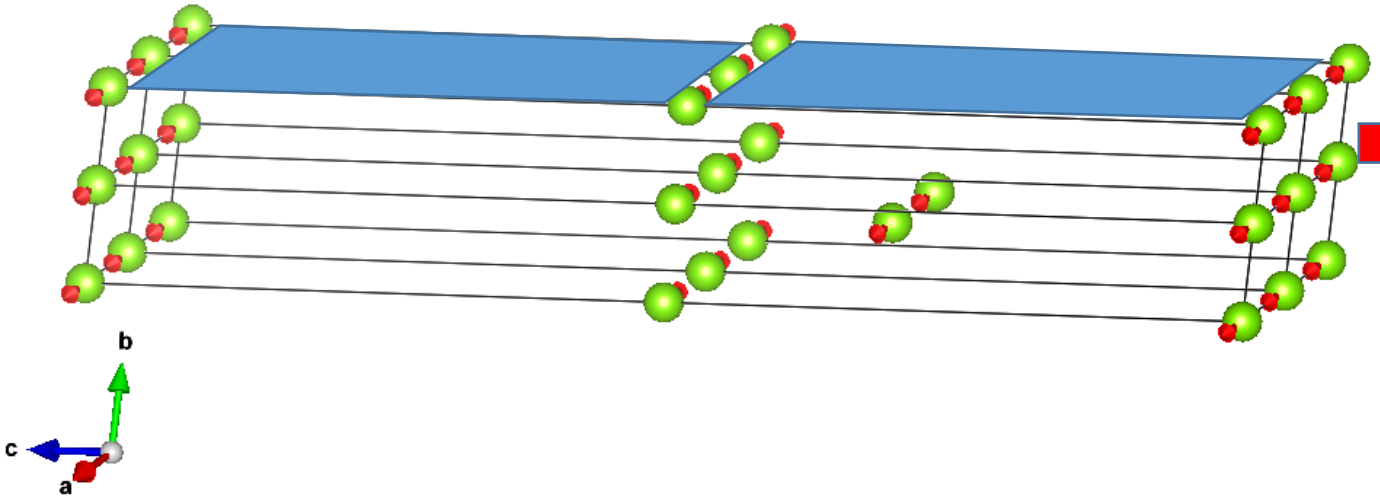
Topological Surface States

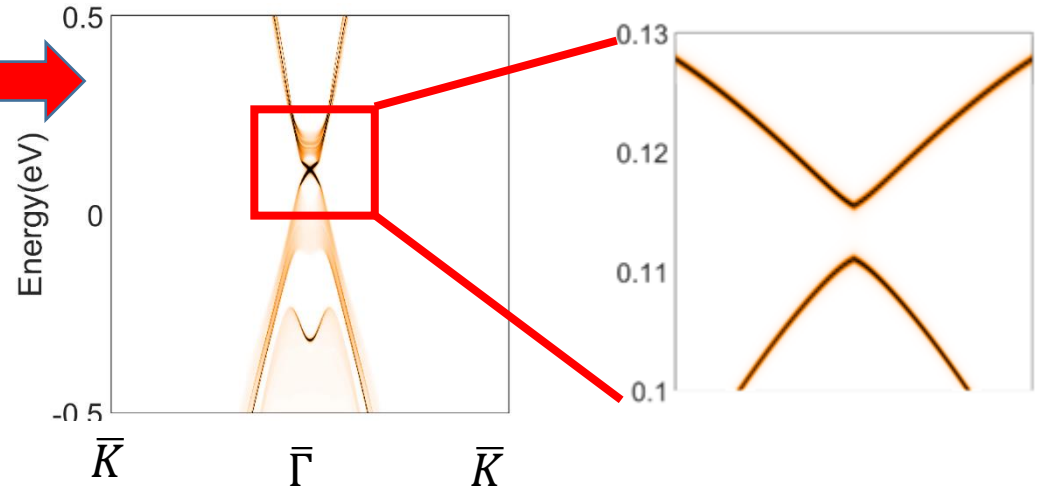




(010) plane preserves $S = \Theta T_{1/2}$ symmetry

(001) plane





(001) plane doesn't preserve $S = \Theta T_{1/2}$ symmetry

Conclusion

- Based on the definition of the topological invariant Z_2 in antiferromagnetic system, our calculation results indicate that the new synthesized compound $EuSn_2P_2$ is an antiferromagnetic topological insulator.

- The gapless topological surface states exist on the (010) plane , while on the (001) plane these TSS open a gap since the combined symmetry are broken, also these SS on (001) surface are consistent with results from ARPES.

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A New Magnetic Topological Quantum Material Candidate by Design

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Thanks for listening!