

Band Topology in LK-99



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Outline

- Introduction/Motivation
 - LK-99
 - Weyl Semimetals
- Results
 - DFT
 - Model Hamiltonian
- Conclusion

LK-99

Claim on July 22,2023

System : Pb-Cu-P-O

The First Room-Temperature Ambient-Pressure Superconductor

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[S. Lee et al., arXiv preprint arXiv:2307.12008 \(2023\).](#)

Superconductor $\text{Pb}_{10-x}\text{Cu}_x(\text{PO}_4)_6\text{O}$ showing levitation at room temperature and atmospheric pressure and mechanism

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[S.Lee at al.. arXiv preprint arXiv:2307.12037 \(2023\).](#)

Validity ??

SUPERCONDUCTIVITY | NEWS

'Room-temperature superconductor' LK-99 fails replication tests

15 Aug 2023 Margaret Harris

nature

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NEWS | 16 August 2023

LK-99 isn't a superconductor — how science sleuths solved the mystery

Efforts to replicate the material have pieced together the puzzle of why it displayed superconducting-like behaviours.

Replication and study of anomalies in LK-99—the alleged ambient-pressure, room-temperature superconductor

T. Habamahoro^{1,2}, T. Bontke^{1,2}, M. Chirom^{2,3}, Z. Wu^{1,2}, J. M. Bao^{2,3,4}, L. Z. Deng^{1,2*}, C. W.

Chu^{1,2*}

- Structural Transition
- Cu₂S impurity

[T. Habamahoro et al. arXiv preprint arXiv:2311.03558\(2023\).](#)

Question?

- Controversy about superconductivity!!
- Is there anything interesting other than superconductivity in LK-99?
 - Band Topology

Weyl Semimetals

- 3D material with non-degenerate band intersections (Weyl nodes)
- Weyl Hamiltonian near each Weyl node,

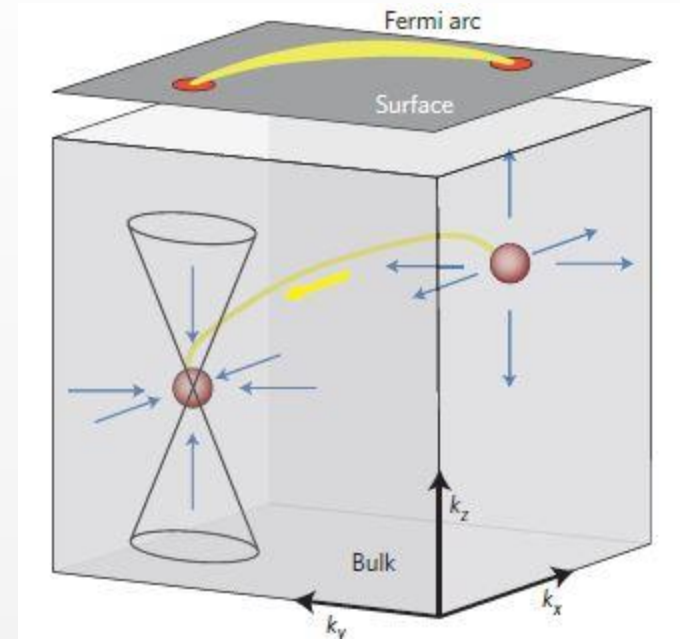
$$H = \hbar v p \cdot \sigma \quad \textcircled{1}$$

- 3D-topological semimetals,
- Chern number

$$C = \int_k \Omega \cdot da$$

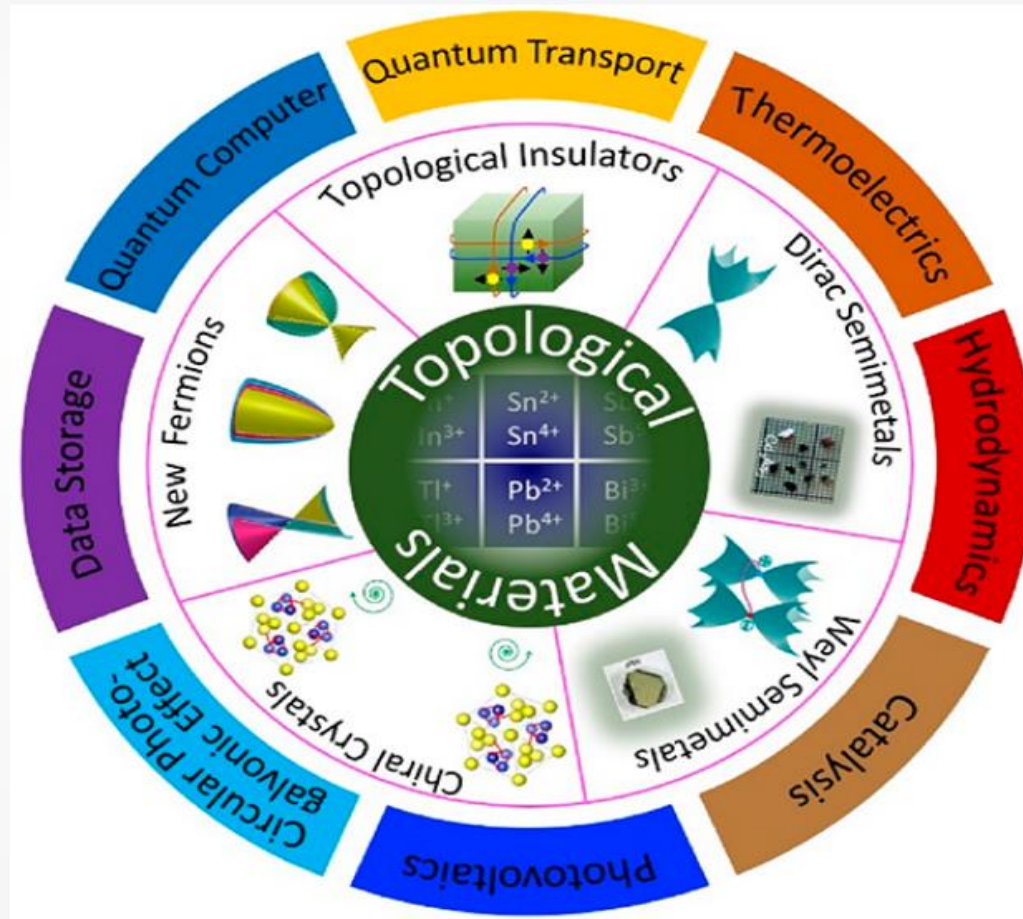
$$\Omega = \nabla \times A \quad \textcircled{2}$$

- $C = \text{integer}$
- Fermi arc states



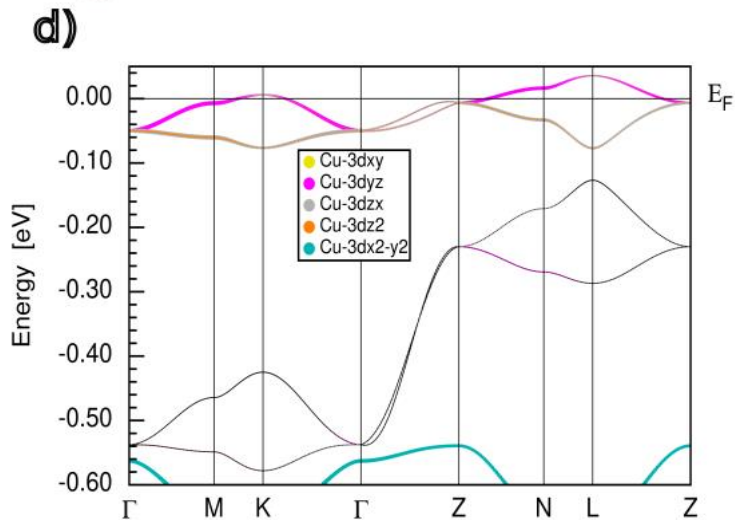
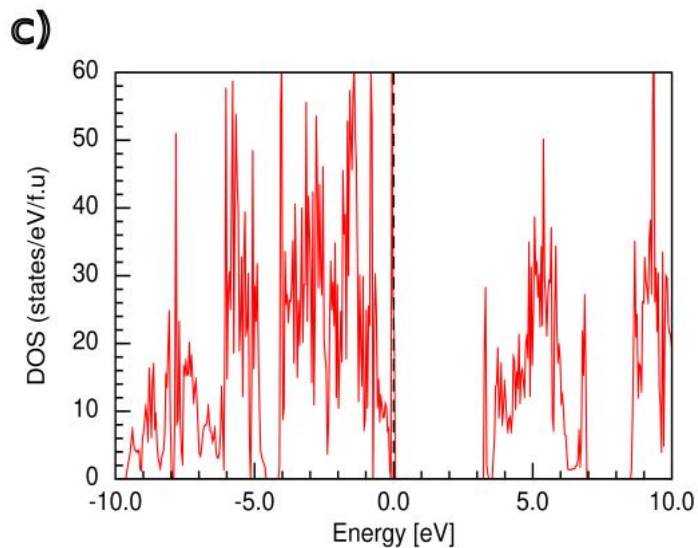
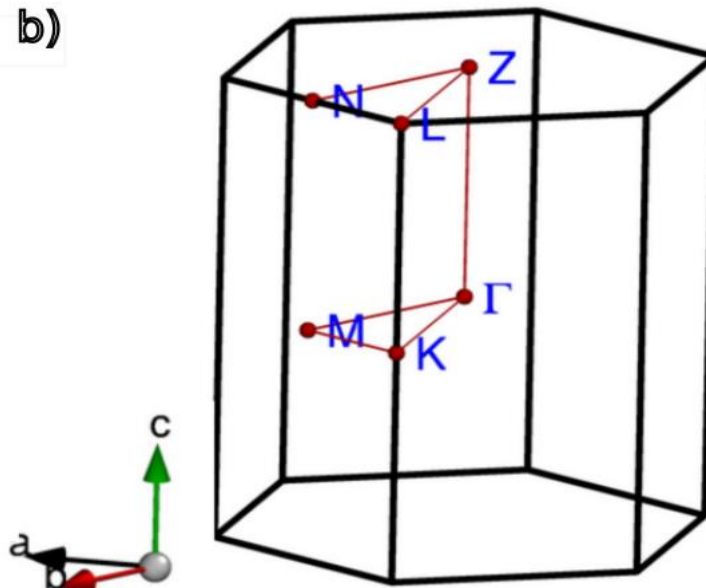
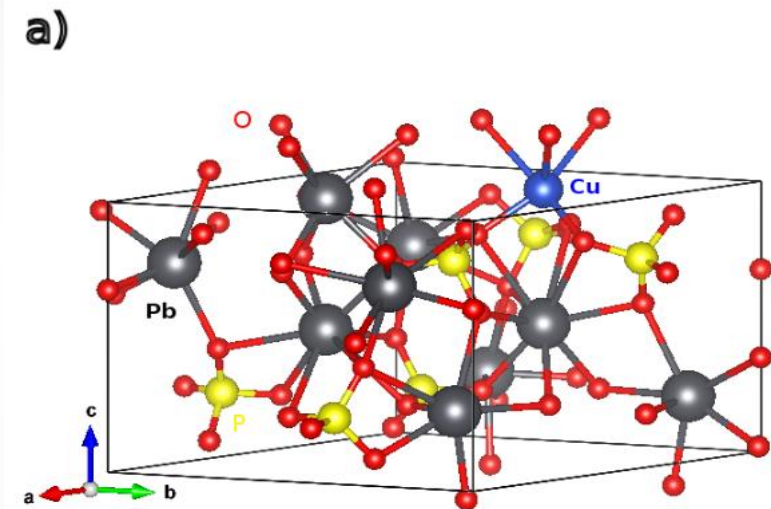
Applications/Motivations

N. Kumar *et al.*, Chem. Rev. 121, 2780 (2021)



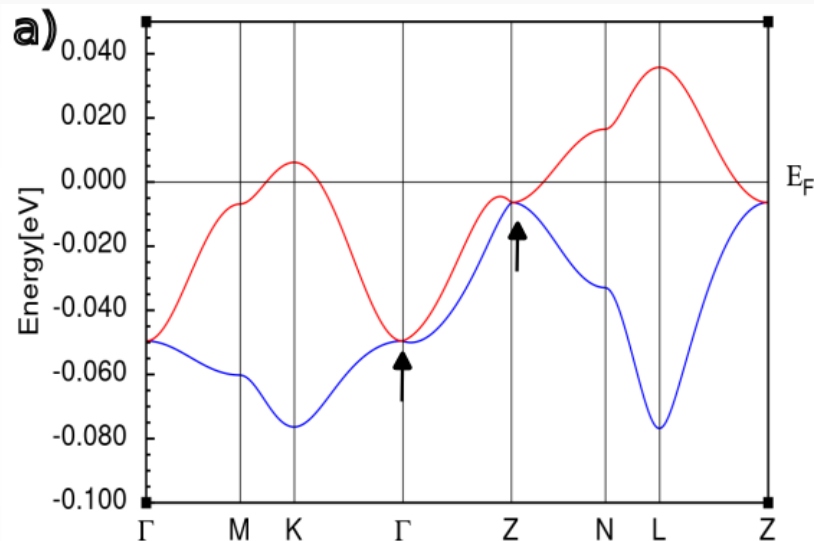
Can we expect any of the topological phase in LK-99?

Crystal Structure and Electronic Features

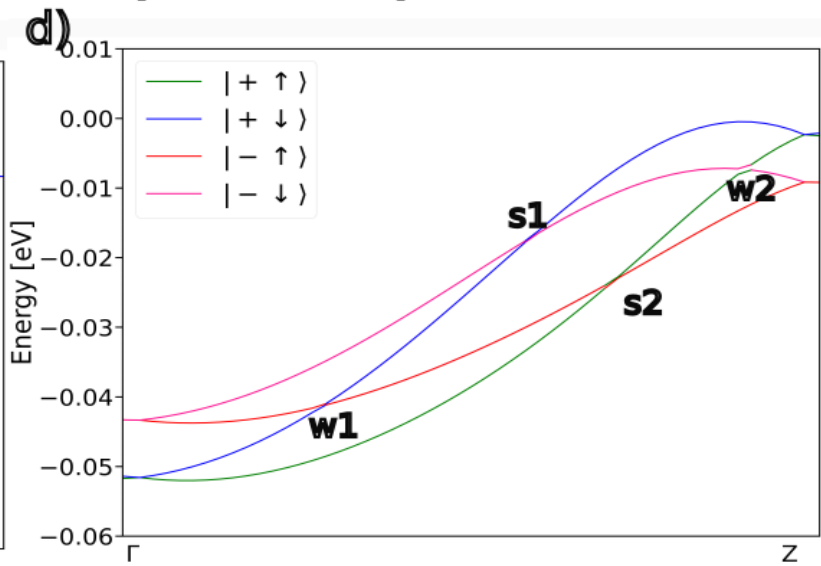
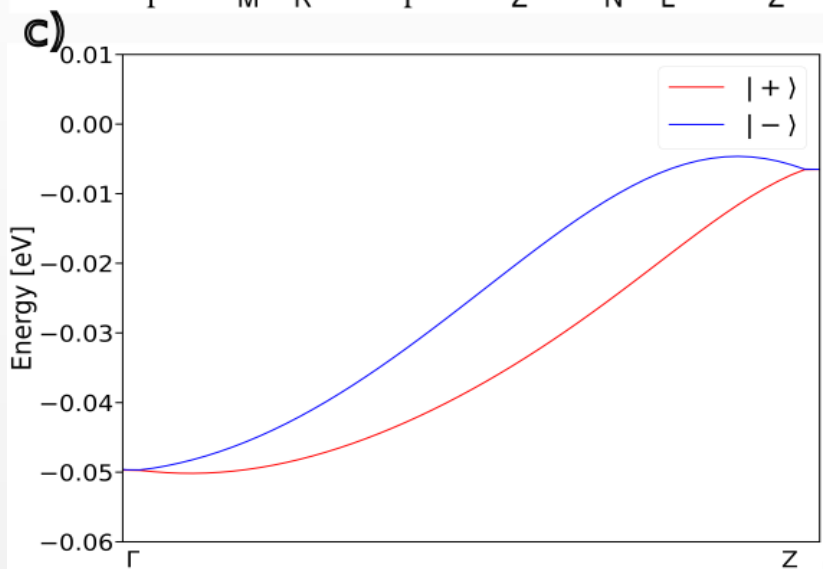
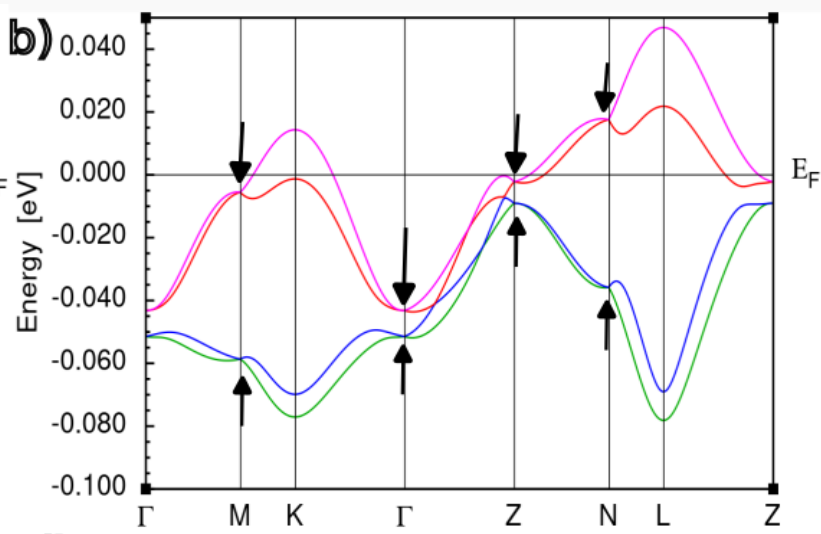


Band Structure: DFT Results

w/o SOC



SOC



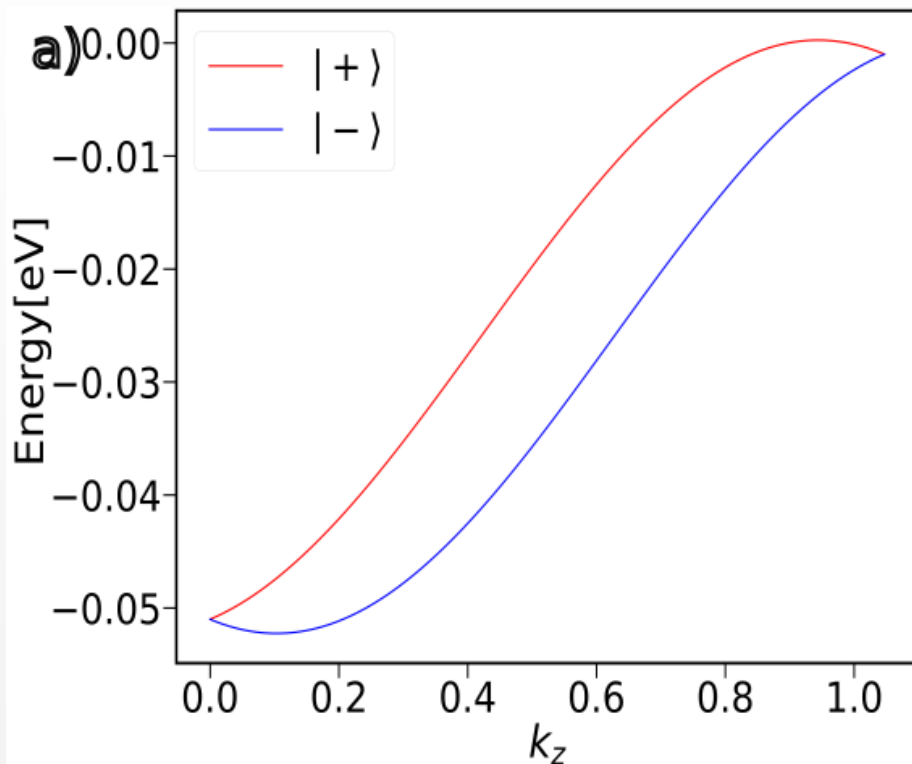
Model Hamiltonian

$$H = H_0 + \frac{\lambda}{2} \tau_z \otimes \sigma_z ; H_0 = \begin{pmatrix} h_+ & h_{+-} \\ h_{-+} & h_- \end{pmatrix}$$
$$H = H_0 + H_{SOC}$$

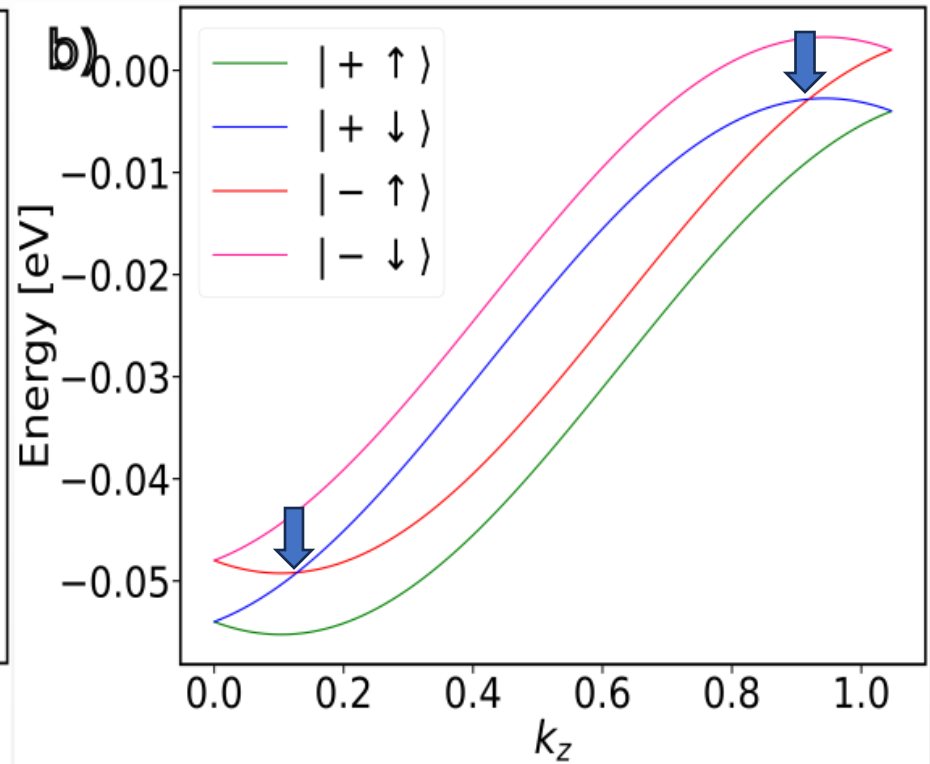
3

B. T. Zhou and M. Franz, arXiv preprint arXiv:2308.07408 (2023).

w/o SOC



SOC

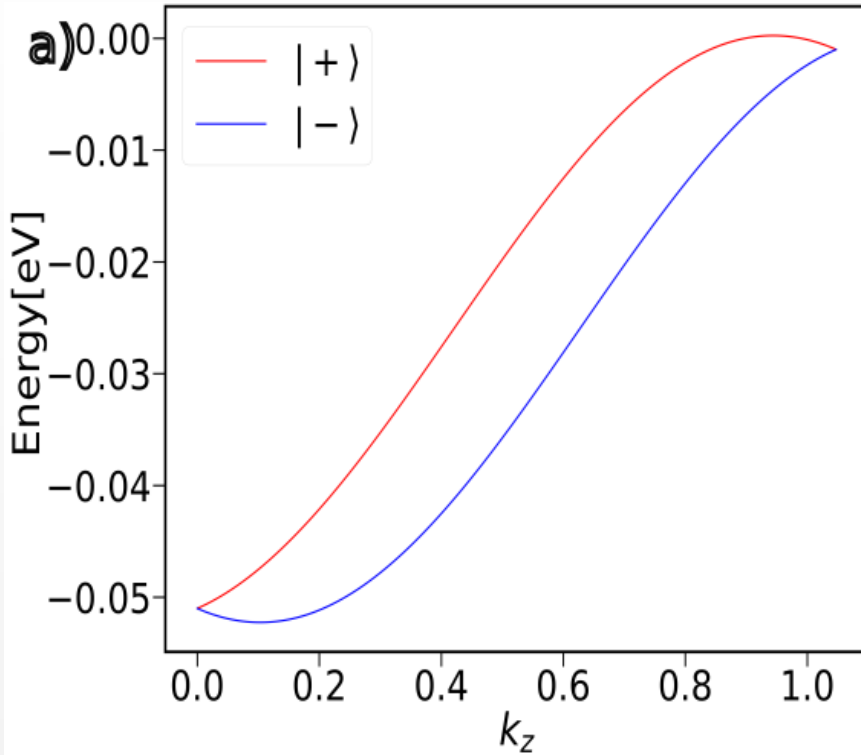


Augmented Model Hamiltonian

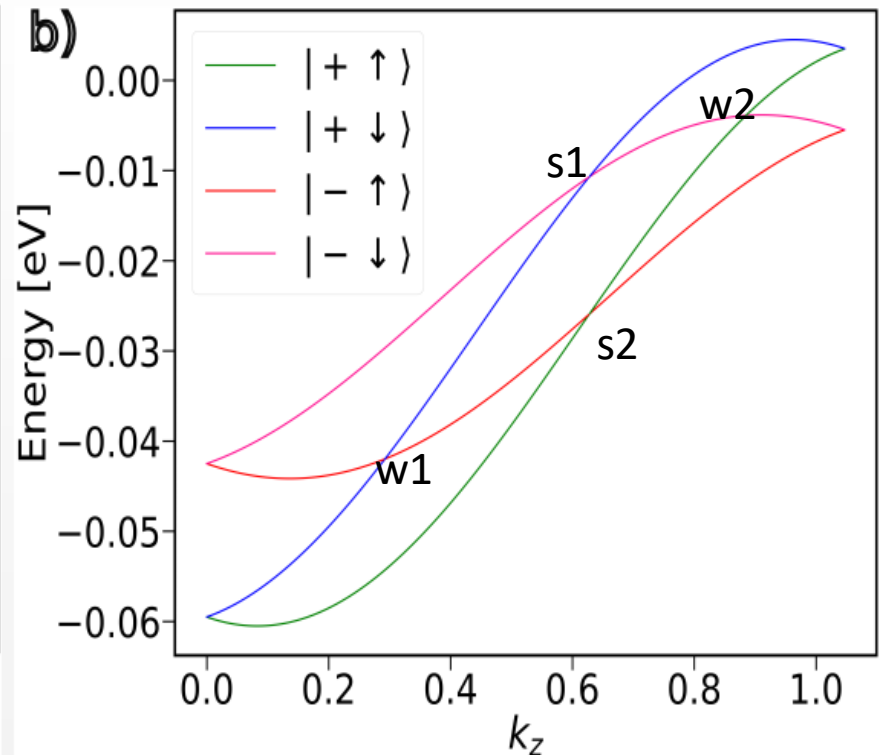
$$H = H_0 + \frac{\lambda}{2} \tau_z \otimes \sigma_z + \frac{\lambda'}{2} \cos(k_z c) \tau_z \otimes \sigma_z$$

4

w/o SOC



SOC



Weyl Points

w1 & w2

$$H_{w1,w2} = a(k_x^2 - k_y^2) \boldsymbol{\tau}_x + 2ak_x k_y \boldsymbol{\tau}_y + bk_z \boldsymbol{\tau}_z + ck_z^2 \boldsymbol{\tau}_z$$

5

$$H_{w1,w2} = f_x \boldsymbol{\tau}_x + f_y \boldsymbol{\tau}_y + f_z \boldsymbol{\tau}_z$$

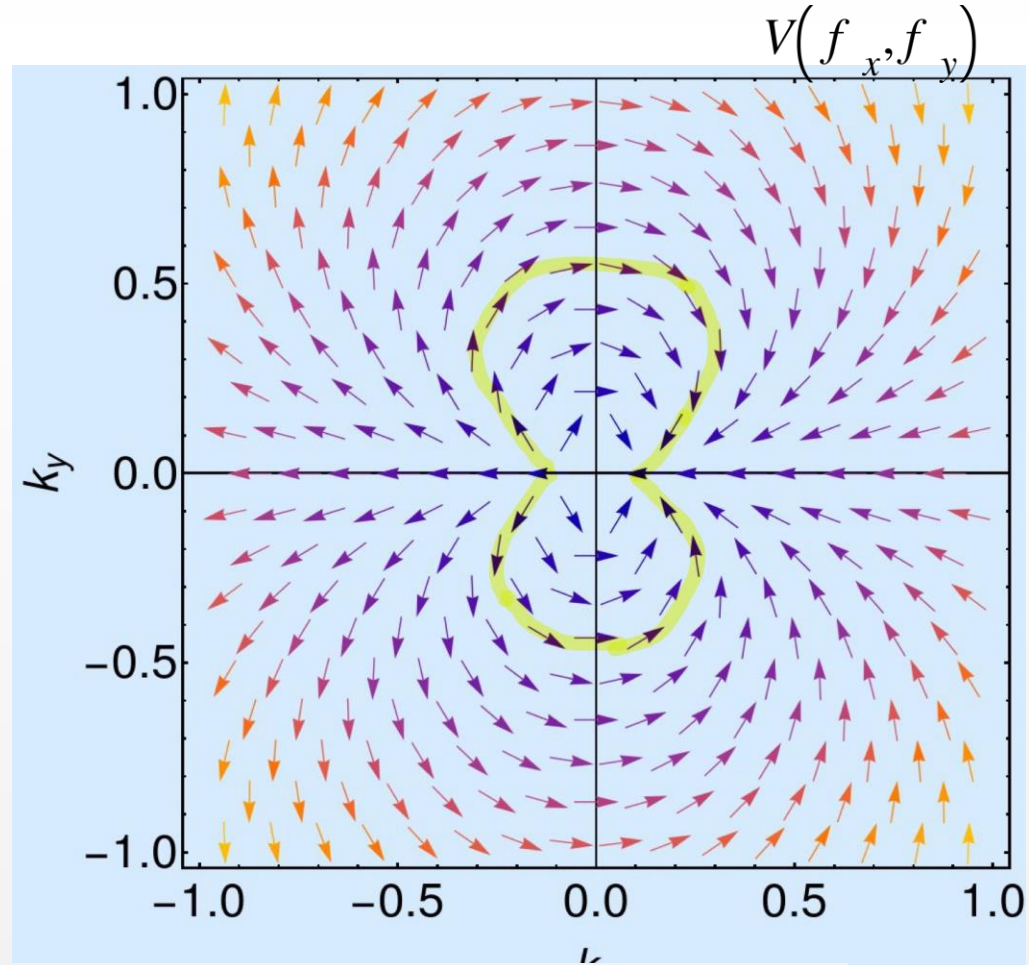
6

$$C_{w1,w2} = 2 \operatorname{sgn}(a) \operatorname{sgn}(b)$$

7

$$C_{w1,w2} = \pm 2$$

8



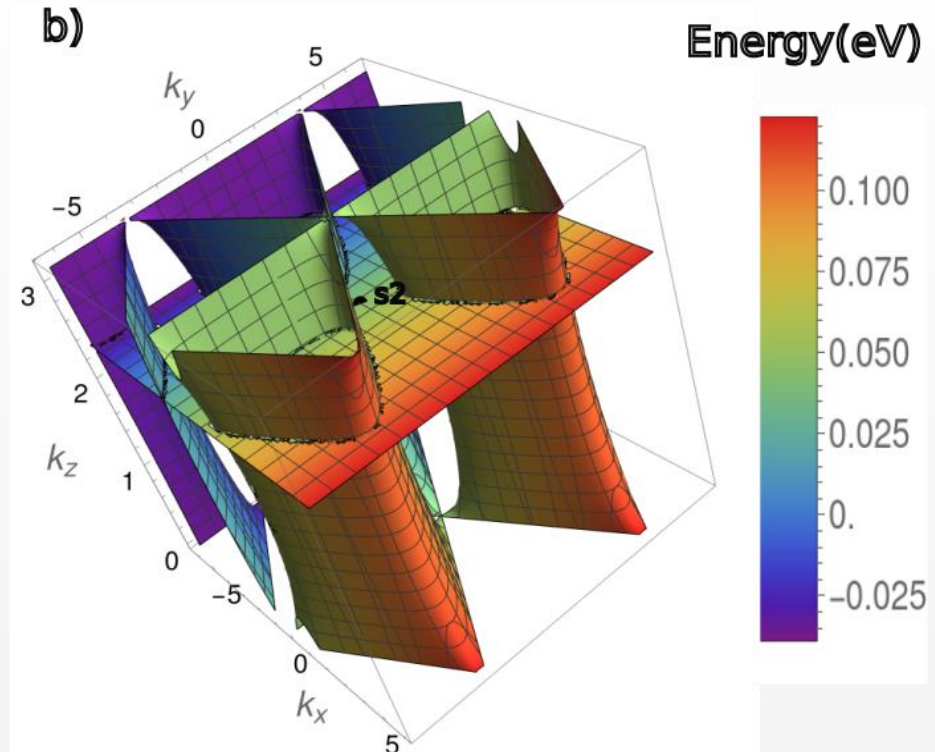
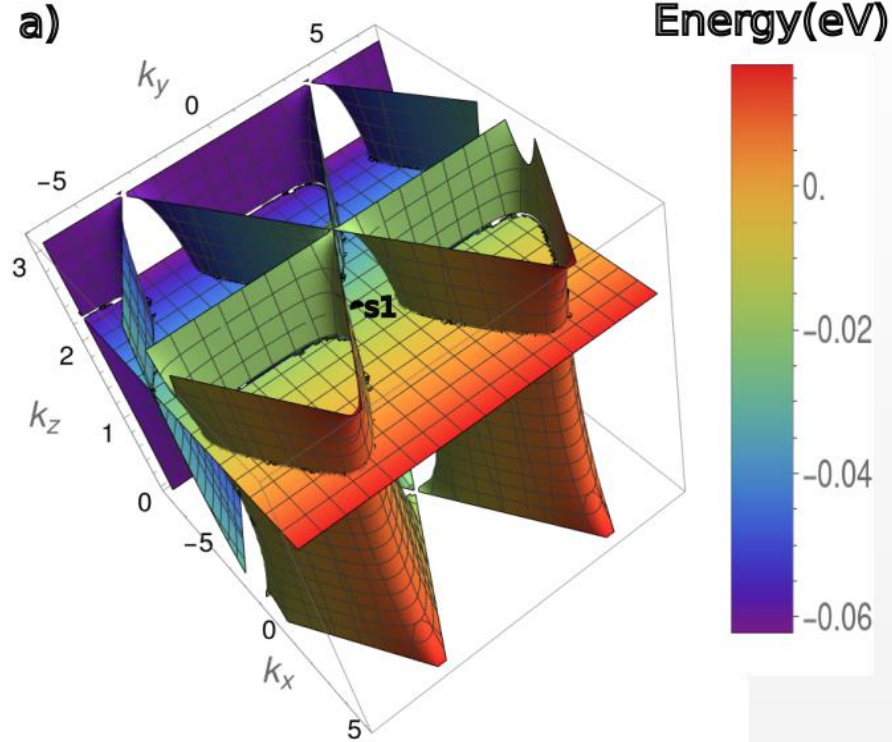
Nodal Surfaces

s1 & s2

$$H_{s1,s2} = bk_z \tau_z + ck_z^2 \tau_z$$

9

$$C_{s1,s2} = 0$$



Conclusion

- LK-99 has interesting band topology
 - Topological Weyl Points
 - Trivial Nodal Surfaces
- SOC plays a crucial role to understand band topology

Acknowledgement

1. Dr. Pavan Hosur
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Thank You