Novel Topological Weyl Semimetallic Phase in Layered Material : Fe_3Sn

Crystals 2020

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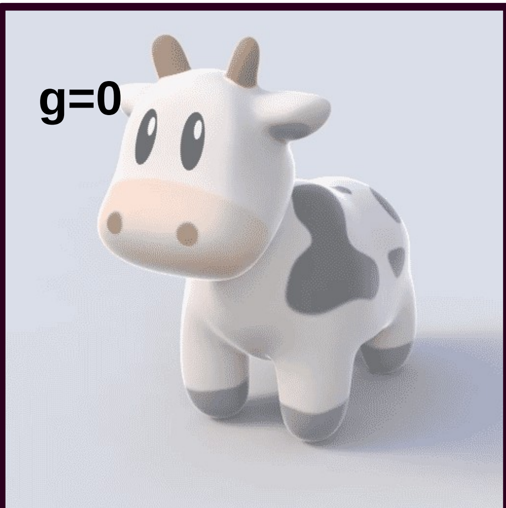
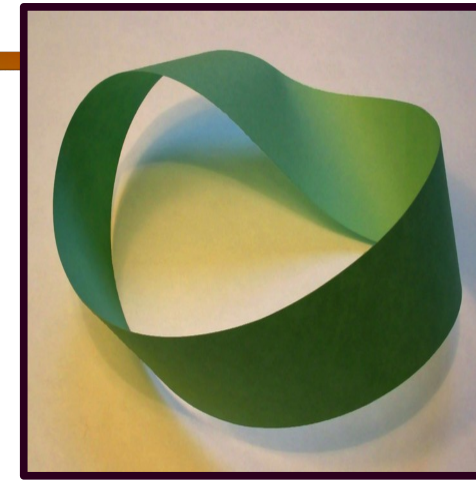
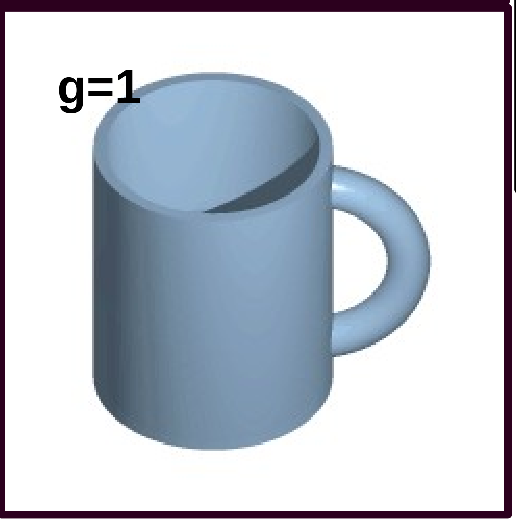
What is Topology ?





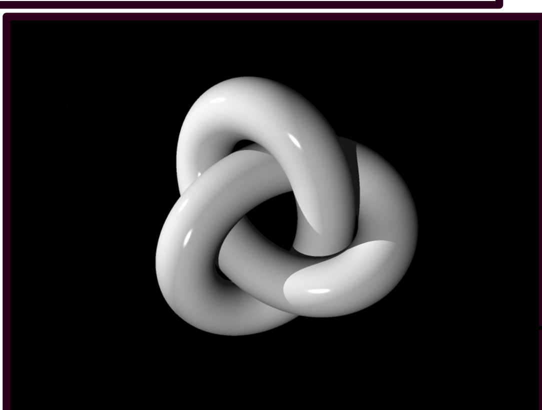
Topology: Branch of mathematics aiming to identify properties of various objects under continuous deformations [1].



Gauss Bonnet- Theorem: Integrate curvature over surface area gives the result as integer.

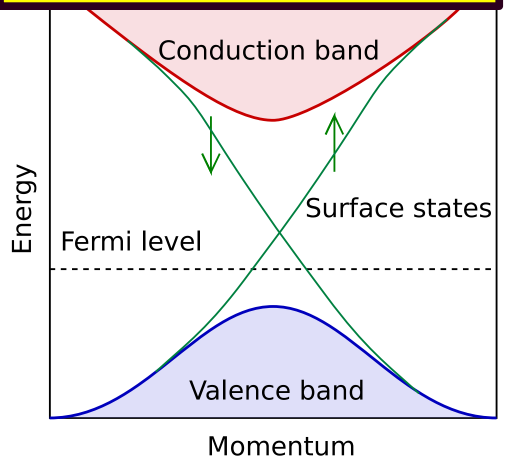
$$\frac{1}{2\Pi}\int_{T^2} K dA = 2-2g \quad \ldots\ldots\ldots\ldots\ldots (1)$$

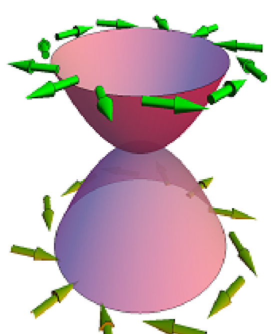
The curvature can be changed locally, but the net integrated value remains constant.



[1] https://en.wikipedia.org/wiki/Topology

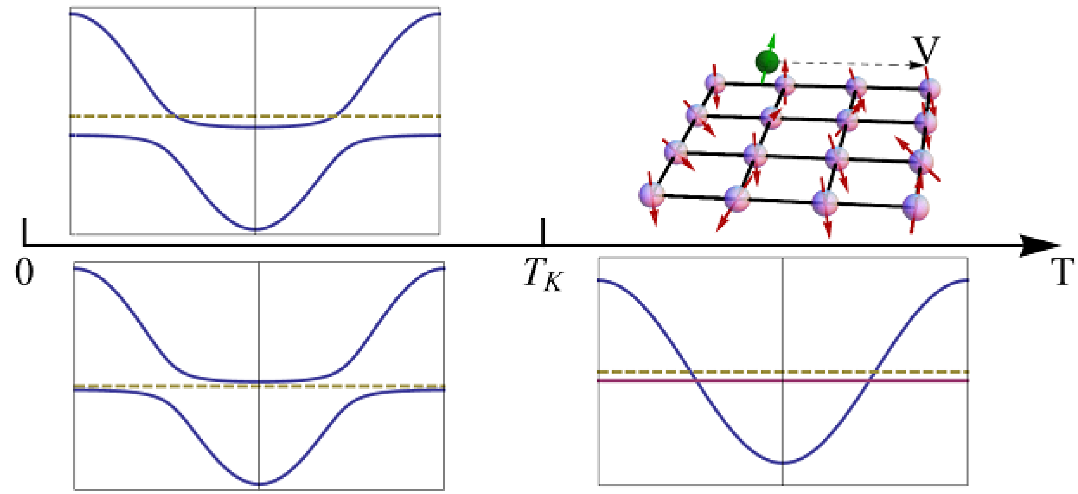
Topological Insulator





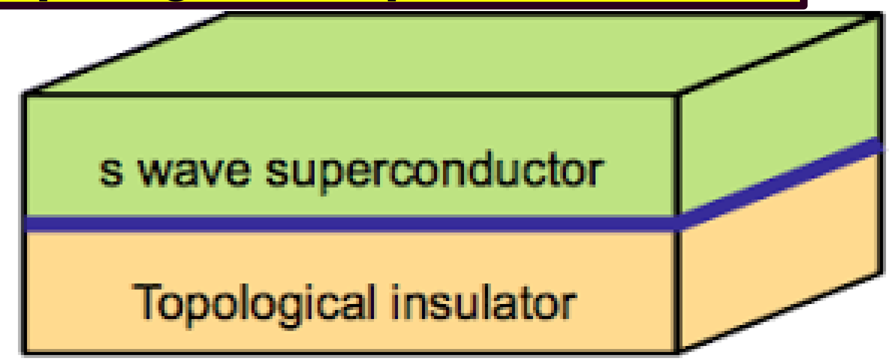
Hasan *et al.*,*RMP*,**82**, 3045(2010)

Kondo Insulator

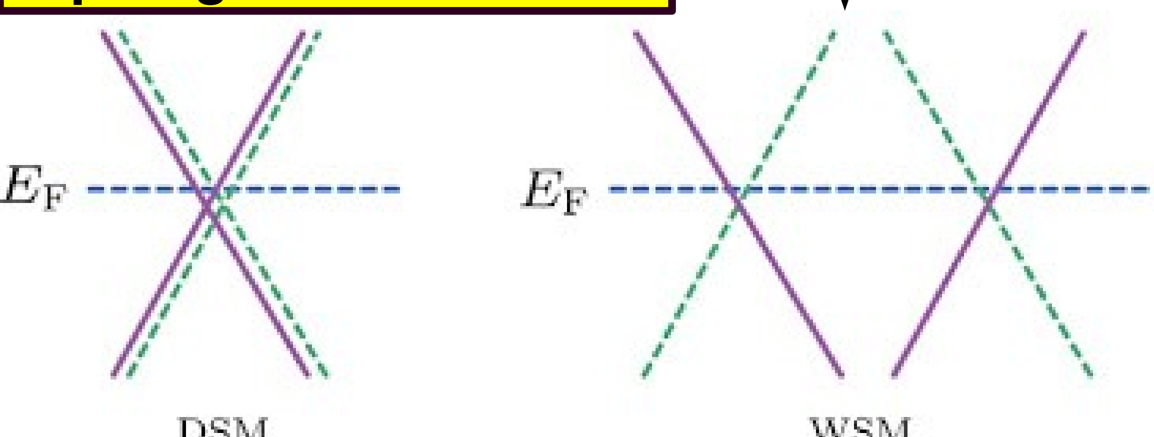


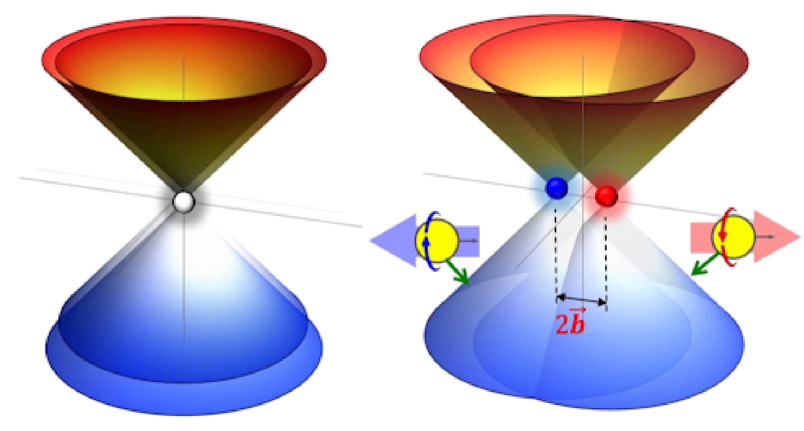
Topological Materials

Topological Superconductors



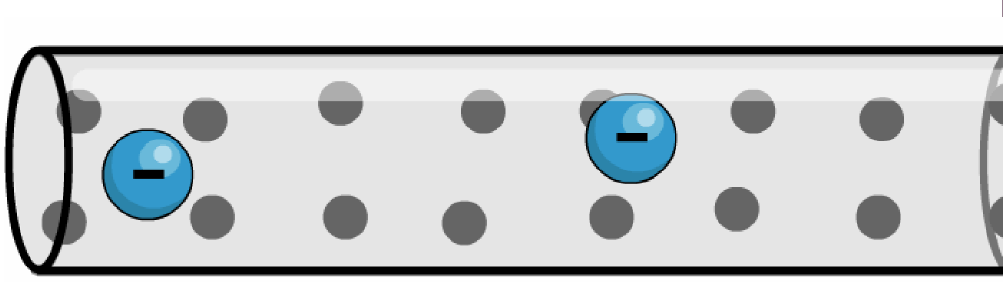
Topological Semimetals



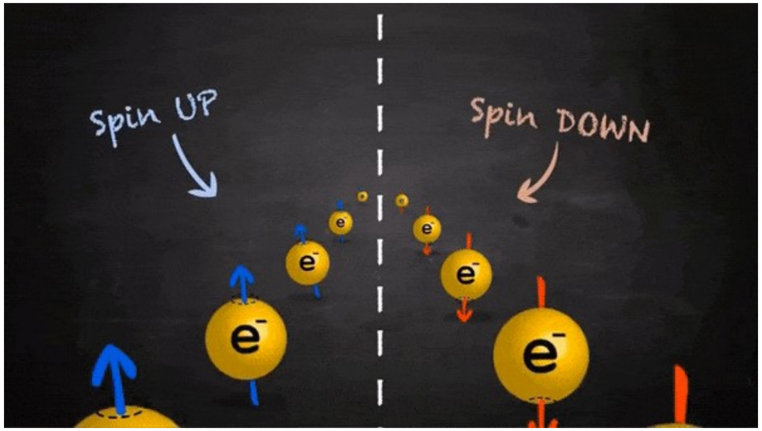


Why to study Topology ?

- **Drawbacks of Electronics**
  - Slow – information carrier is electron having mass and charge
  - Conduction through bulk : Loss of huge amount energy in the form of heat
  - Based on classical bit (0 and 1)



- **Probable Solutions**
  - Fast – Fermi arc transport
  - Conduction through surfaces preserves huge amount of heat loss
  - Quantum bit



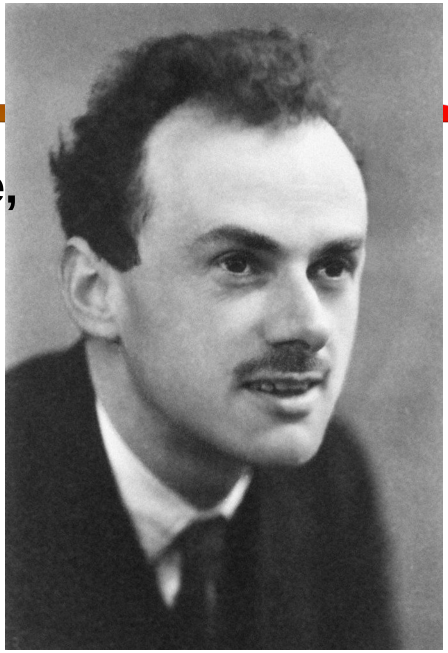
Dirac and Weyl Equations

- Dirac introduced linearized momentum for relativistic free particle,

$$H_D = E = c\,\vec{\alpha}.\vec{p} + \beta m c^2 \text{..............} (2)$$

- α and β are terms introduces to satisfy special theory of relativity and Pauli principle,
- Introducing 4 X 4 Gamma matrices , 1929 Dirac Equation ,

$$\begin{pmatrix} E(\vec{k}) - \sigma.\vec{k} & 0 \\ 0 & E(\vec{k}) + \sigma.\vec{k} \end{pmatrix} \psi = mc^2 \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix} \text{...........} (3)$$



P. Dirac

- The solution gives four folded Dirac Points.
- Dirac Points: Sources for Dirac Fermions
- Weyl solved the Dirac equation setting the mass to zero.
- Weyl equation 1930, 2X2 Matrix equation,

$$i\partial_t \Psi_{\pm} = H\,\Psi_{\pm} = \pm\vec{k}.\vec{\sigma}\,\Psi_{\pm} \text{...........} (4)$$

H. Weyl

- The solution gives two folded Weyl points with definite Chirality
- Weyl Points: Sources for Weyl Fermions

Weyl Semimetals

- Weyl semimetals (WSMs) are the crystalline substances which are the sources for the Weyl fermions.
- Breaking of TRS or IS or both results crossing of valance and conduction band creating Weyl node.
- The Weyl node:
  - Follows Weyl equation.
  - Can act as magnetic monopole
  - Source for Berry Curvature
  - Fermi arc states between two Weyl nodes
- WSMs exhibit high mobilities, magnetotransport phenomenon and large magnetoresistance.
- There are mainly two types of WSMs:
  - Type I : Lorentz violating, direct crossing in *k* space, nodal line and plane are perpendicular
  - Type II : Lorentz invarient, indirect band gap in *k* space, nodal line and plane makes some angle

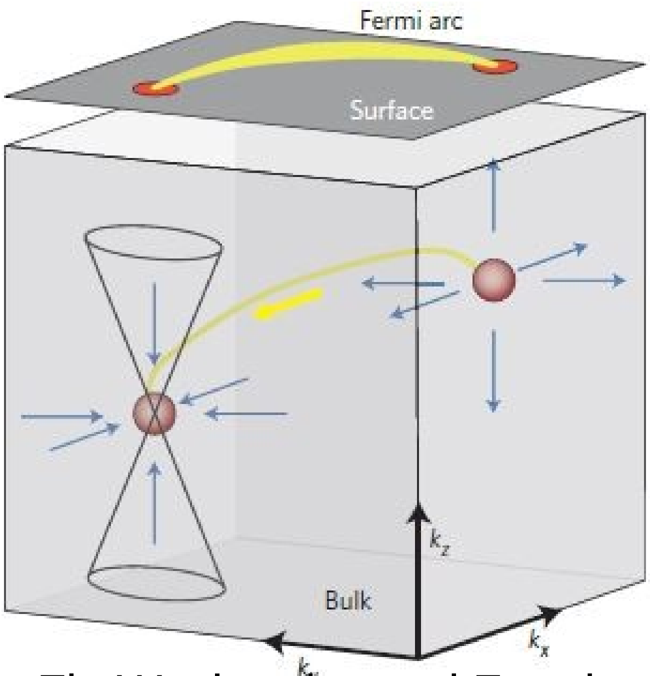


Fig:Weyl nodes and Fermi Arc States [1]

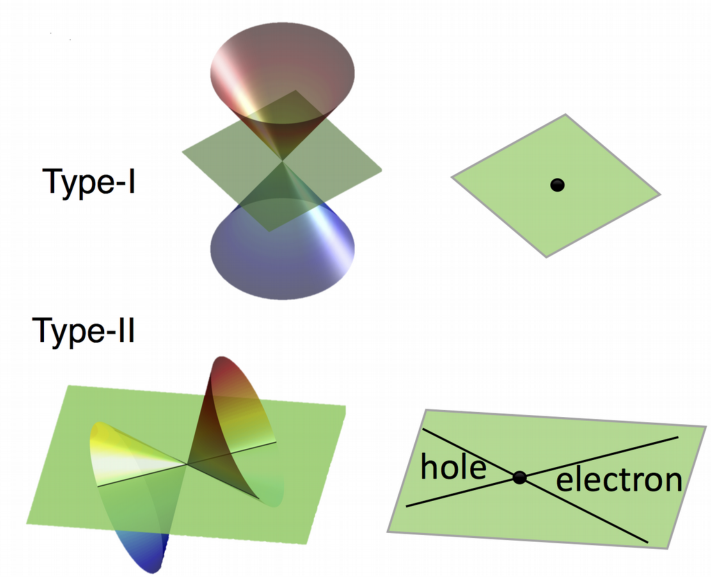
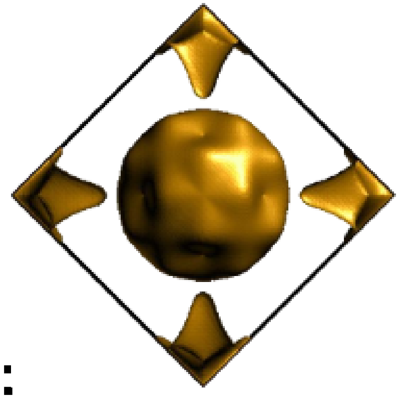


Fig:Types of WSMs [2]

[1] Bernevig *Nat. Phys*. **11**, 698 (2015)
[2] Felser et al., *ARCMP*, **8**, 337 (2017)

Computational Approach

- **Full potential local orbital minimum basis code (FPLO) is used which is based on Density functional theory (DFT) approach**



- **DFT formalism**
    - **Electronic Properties**
    - **Magnetic Properties**

- **Wannier Interpolation and Berry Phase Formalism:**
    - **Topological Properties**
    - **Weyl Properties**
    - **Chern Numbers**
    - **Anomalous Hall effects**

Crystal Structure: Fe_3Sn

- **Layered Material**
- **Hexagonal crystal**
- **Kagome System**
- **Space Group No: 194 (*P63/mmc*)**
- **Point Group D6h with 24 full group operations**
- **Non Symmorphic**
- **Breaks Inversion Symmetry**
- **Candidate for Weyl Semimetals**
- **Lattice Constants: $a=b= 5.487$ A^o $c= 4.310$ A^o**
- **$\alpha=\beta= 90^o$, $\gamma=120^o$**

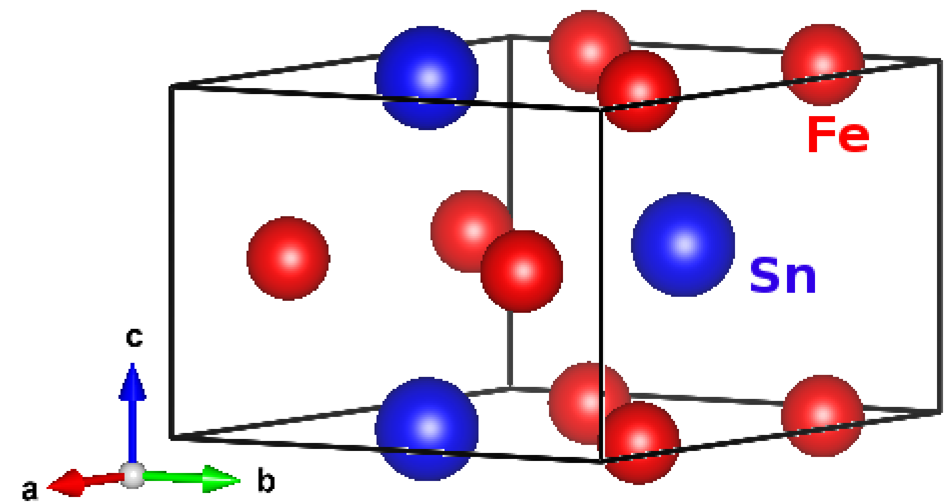


Figure. Crystal Structure

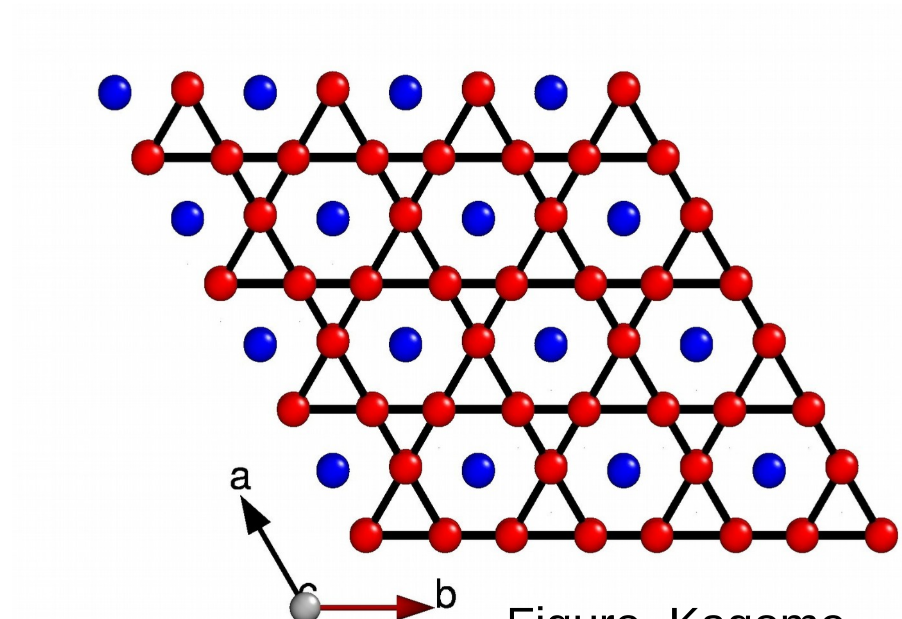
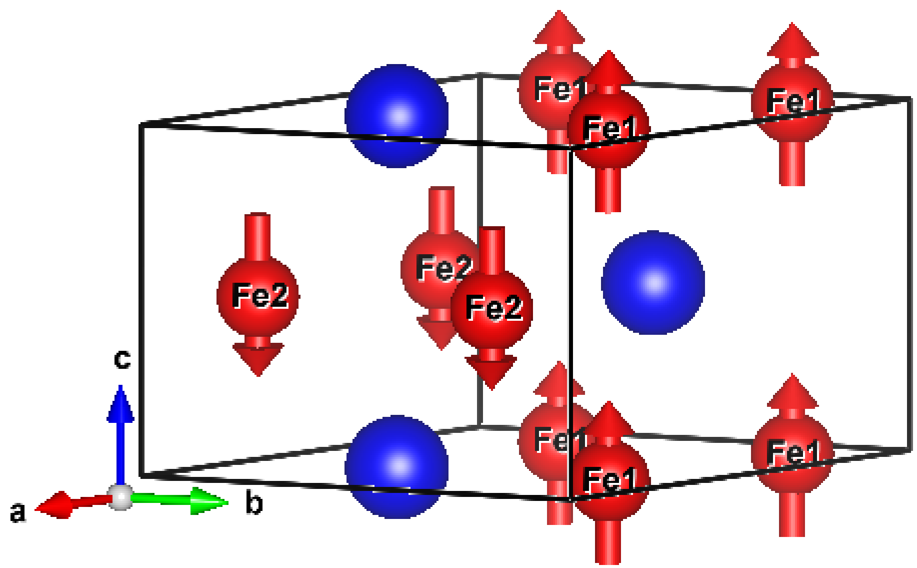
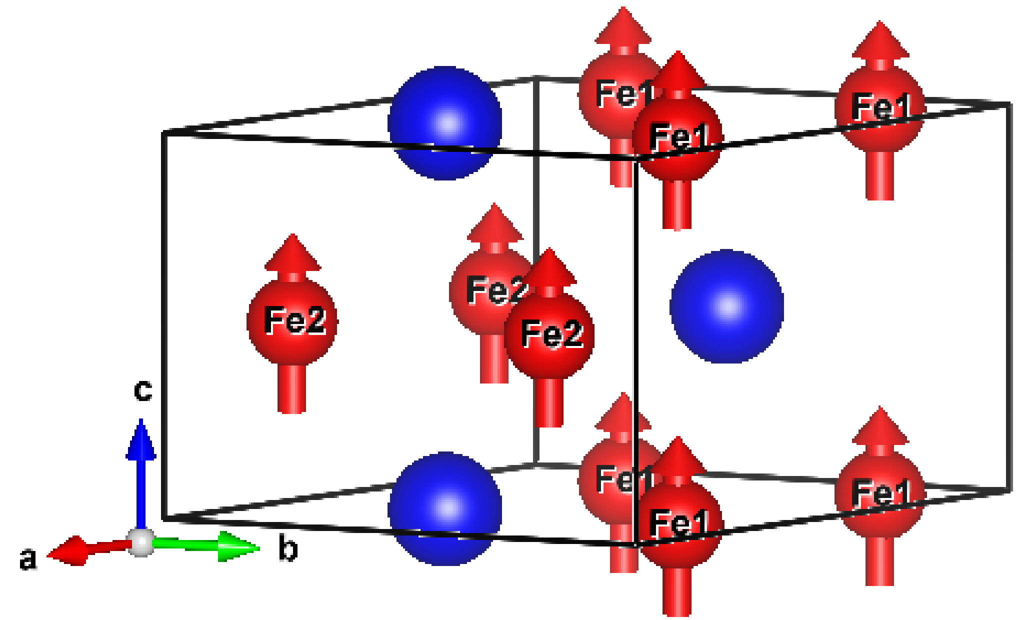


Figure. Kagome Structure

Magnetic Ground State



AFM

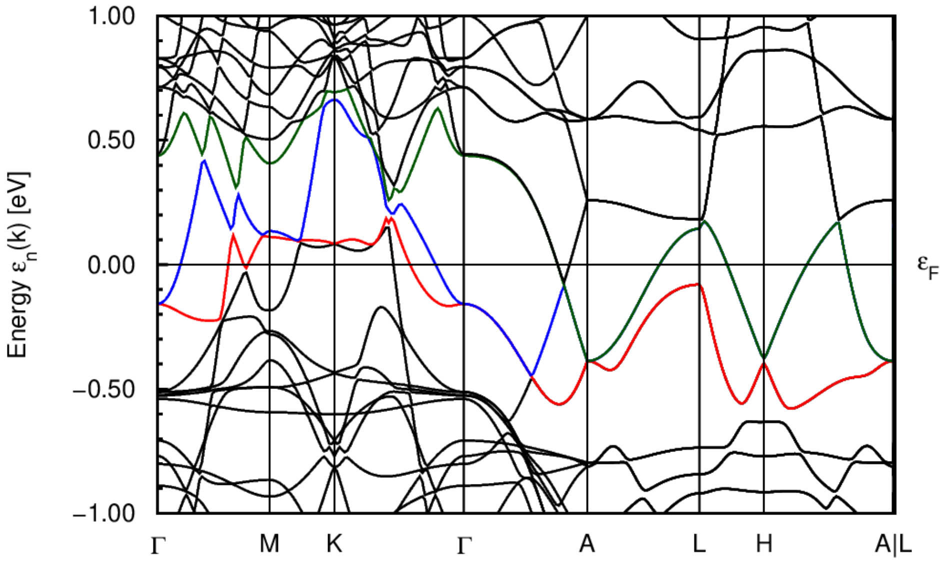


FM

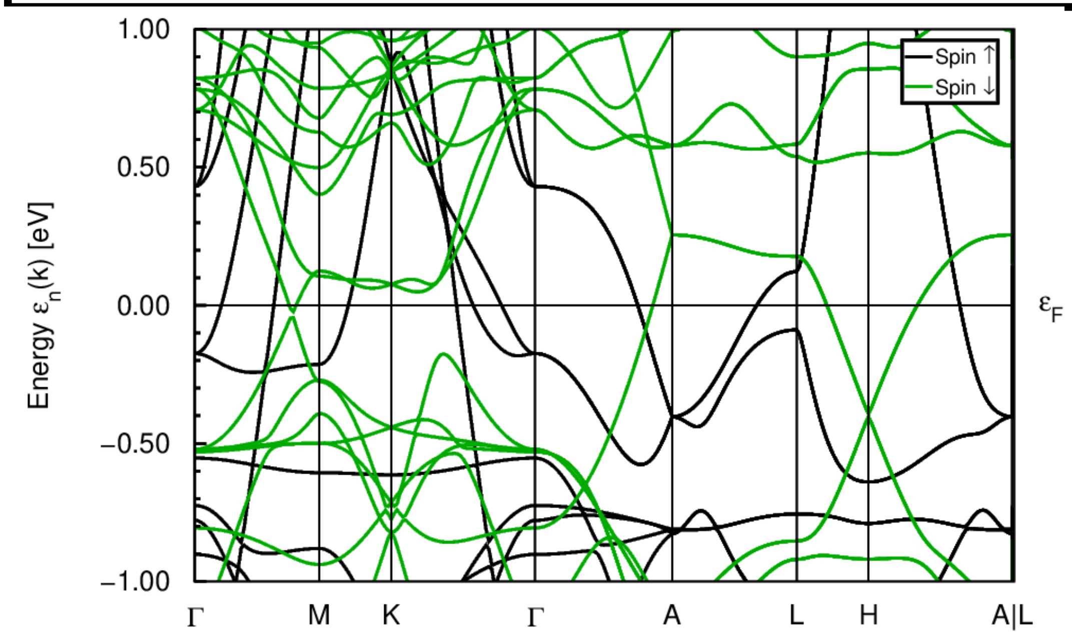
- **Two magnetic configurations are possible from the spin texture configuration**
- **Fe1 and Fe2 : ↑↓ for AFM and ↑↑ for FM**
- **FM ground state is observed**
  (Magnetic compound breaks Time Reversal Symmetry suitable for Weyl Phases)

Electronic Band Structures

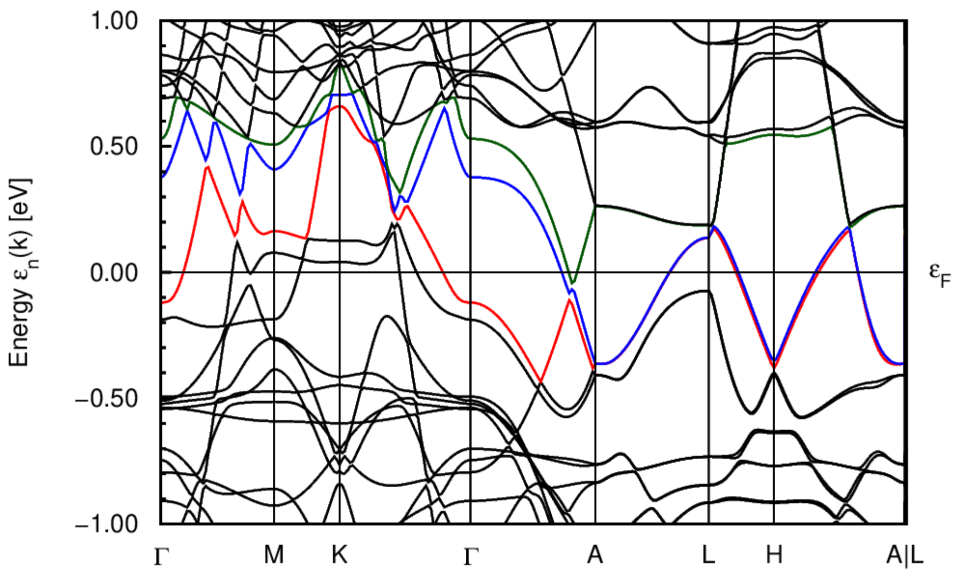
- **Presence of heavy atom Sn shows SOC effects in band structure**
- **Degenerate bands open to form non degenerate bands**
- **Crossings at the Fermi level: Weyl Indication**
- **Magnetic Anisotropic Effects**
- **$E_{001} - E_{100} = 1.08$ meV**



SOC (100)



Without SOC



SOC (001)

Contribution of States

- **No band gap around Fermi level : Metallic in nature**
- **Major contribution of Fe- 3*d* orbital and minor contribution from Sn – 5*p***
- **These orbitals plays role for Weyl point formation**
- **Flat nature around -0.5 eV mainly contributed by d_{yz} and d_zx**
-

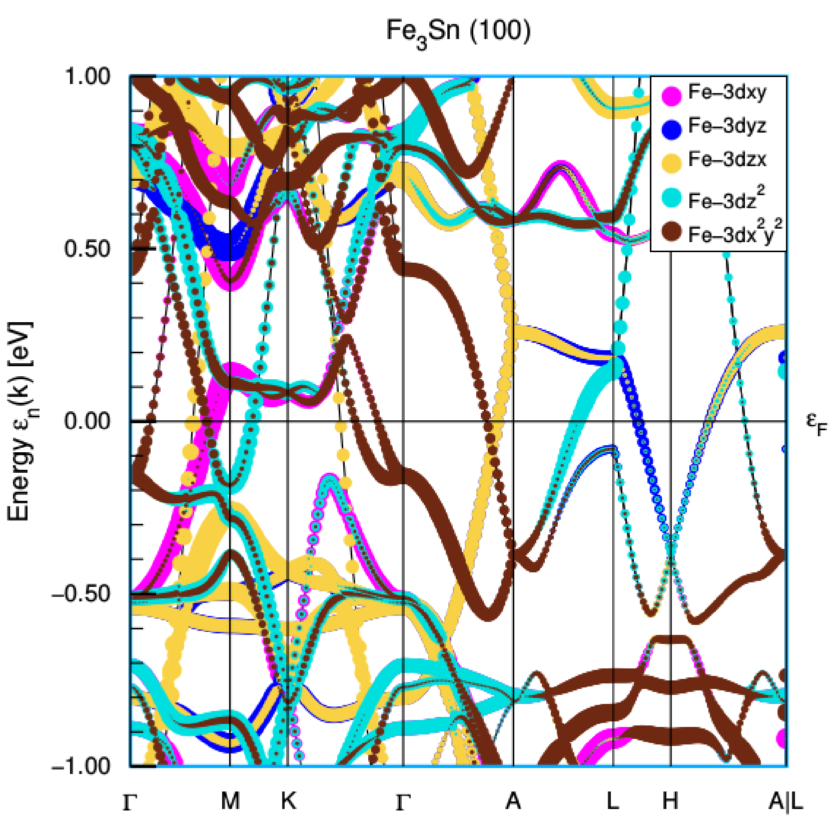


Fig: Contribution of Fe-3*d* and Sn-5*p* states in band structure

Weyl Points

- Wannier Fitting : Matching of DFT band, Wannier band and Tight band approximation

- Generation of Wannier Hamiltonian

- Weyl points are identified using Berry Curvature Formalism
- Chern Numbers or Chirality of nodes

- **Along 100 (easy axis)**

Weyl Points	Energy(eV)	Chirality (χ)
W1	78.1 meV	+1
W2	141.0 meV	-1
W3	202.6 meV	+1
W4	397.8 meV	+1

Conclusions

- Fe_3Sn a layered material with ferromagnetic ground state

- SOC effects and magnetic anisotropic effects prevalent in the system

- Breaking of Time Reversal and Inversion Symmetry creates Weyl Points in the momentum space: Weyl Semimetal

Acknowledgments

- IFW-Dresden, Helmholtzstr-20, 01069 Dresden, Germany
- Condensed Matter Physics Research Center, Butwal-11, Rupandehi, Nepal

Thank You !