# TOPOLOGICAL INSULATORS AND DIRAC SEMIMETALS – SYNTHESIS AND CHARACTERIZATION


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# OVERVIEW

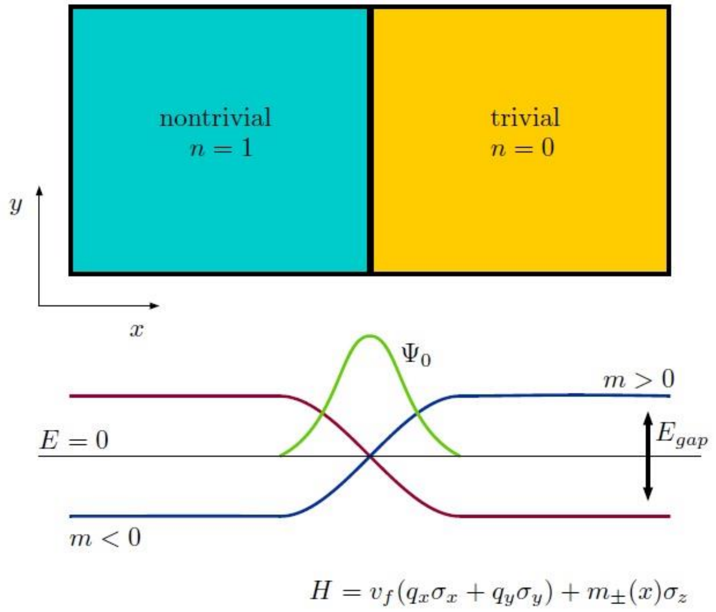
- What are topological insulators and Dirac semimetals?
- Quantum transport and magnetic properties (quantum oscillations).
- Synthesis
- Some concrete materials and measurements.

# TOPOLOGICAL INSULATORS (TI)

**Topological insulator(TI)**

Quantum state characterized by **topological invariant** (nontrivial).

There is an **energy gap**.




Defined over the wave functions (that give the energy gap)

⟹ Invariant under adiabatic change of Hamiltonian.

⟹ The same as long as there is a gap!

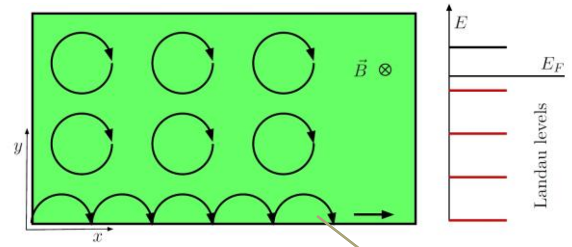
- Closing of the energy gap at the boundary of topological and normal insulator (vacuum)

⟹ conductive edge/surface

# TOPOLOGICAL INSULATORS

- Examples of TI and topological invariant ?

### Quantum Hall effect



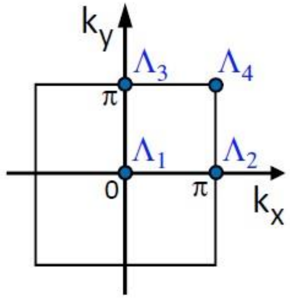

$\sigma_{xy} = n\frac{e^2}{h}, \quad n \in N$ → Edge states

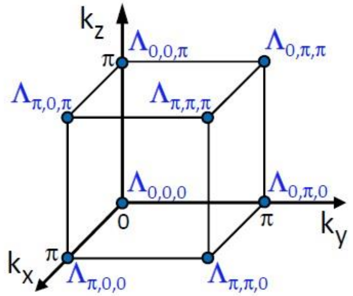
$n$ → topological invariant
(Chern number or TKNN)

~~TRS~~, 2D

### $Z_2$ TI (TRS & IS)

Time reversal operator: $\Theta^2 = -1$




$$2D: \quad (-1)^{\nu} = \prod_{i=1}^{4}\prod_{n=1}^{N} \xi_{2n}(\lambda_i)$$

$\xi_{2n}$ → parity

$\nu = 0,1$ → $Z_2$ topological invariant

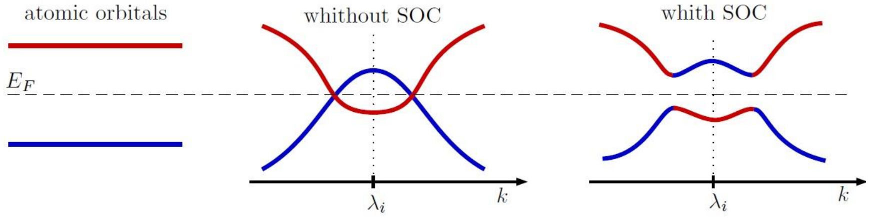
$$3D: \quad \nu_0, \nu_1, \nu_2, \nu_3$$

### Topological crystalline insulator

$\nu = 0$, topological invariant is not determined by TRS but with crystal simmetries (mirror symmetry).

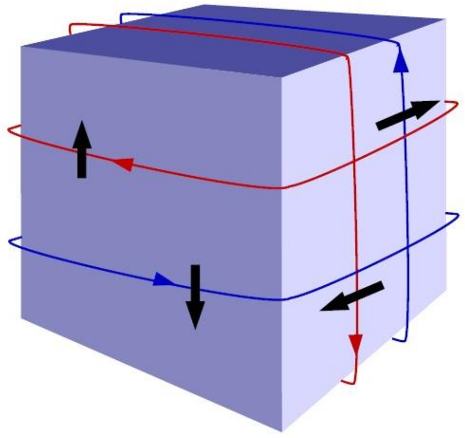
$$M^2 = -1$$

Nontrivial topological invariant if there is an band inversion at some $\lambda$ !




SOC – spin orbit coupling

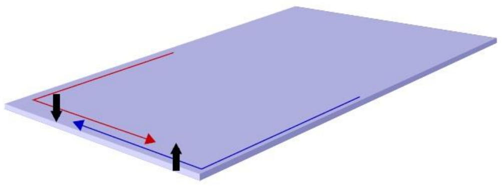
# TOPOLOGICAL INSULATORS

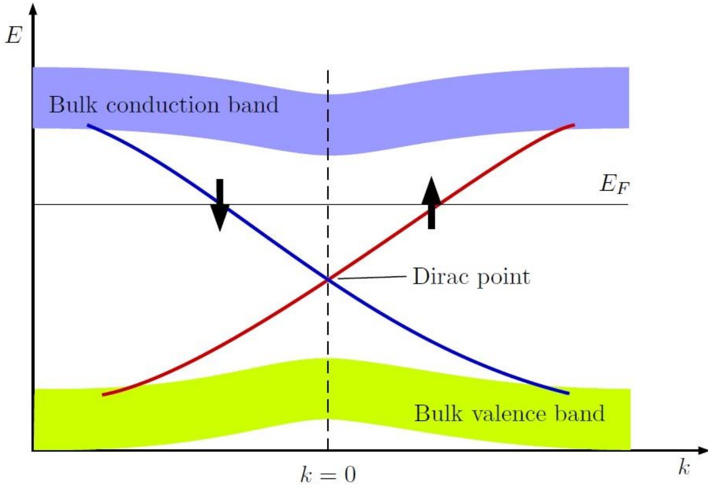


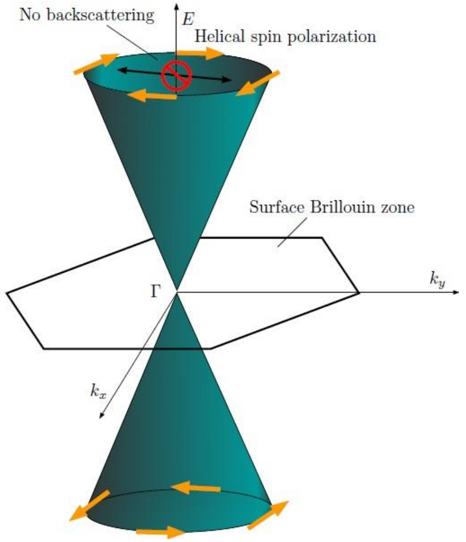
- Edge/surface states properties.

Dirac dispersion in low-energy excitations ⟹ high mobility!

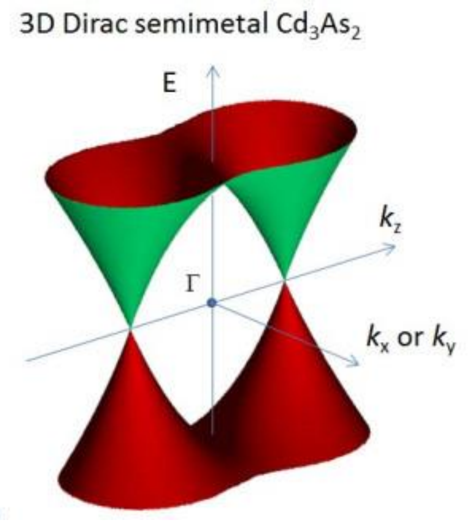
Spin-momentum locking ⟹ forbidden backscattering!





# DIRAC SEMIMETALS





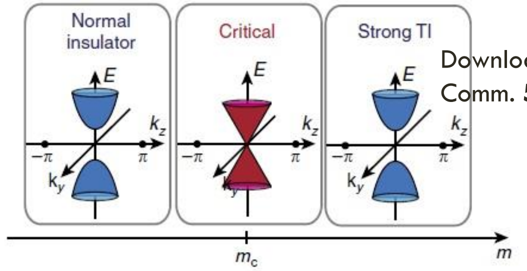

Dirac semimetal

Dirac dispersion in the touch points.

Valence and conduction band touching in discrete points.

- Dirac dispersion in 3D!
- 2D – graphene: $\hat{H}(\vec{k}) = v(k_x\sigma_x + k_y\sigma_y)$ ⟶ SOC ~ $\sigma_z$ opens the gap.
- 3D: $\hat{H}(\vec{k}) = v_{ij}k_i\sigma_j, \quad j = x, y, z$ ⟶ Robust against perturbations!

# DIRAC SEMIMETALS

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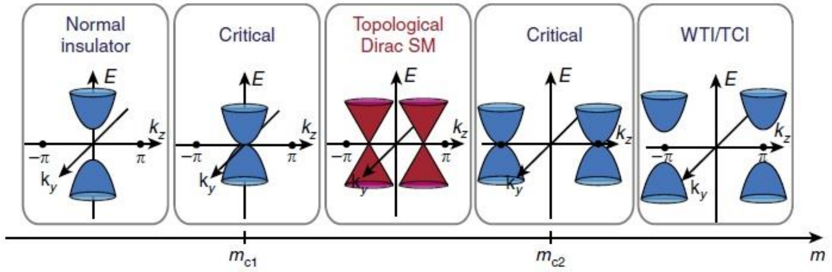
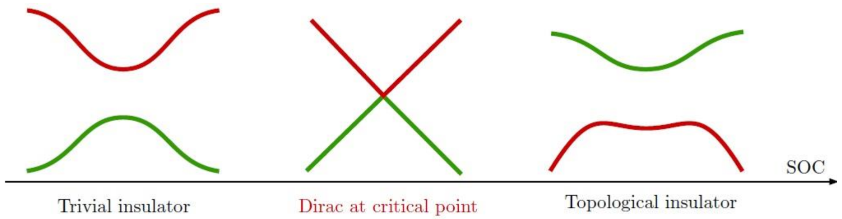
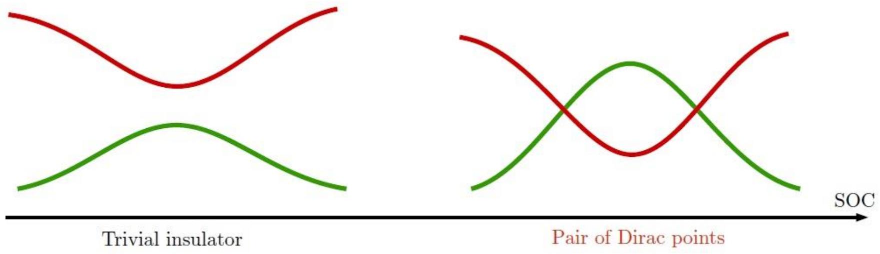



- Dirac semimetals come in two topological clasces too.
  - Consequence of topological phase transition NI – TI.




  - Intrinsic as a result of additional symmetries (rotational symmetry).



# TOPOLOGICAL INSULATORS & DIRAC SEMIMETALS

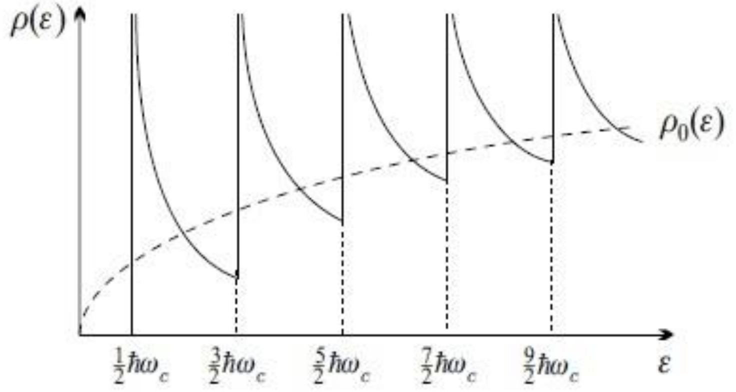
- Topological insulators → 2D Dirac dispersion.
- Dirac semimetals → 3D Dirac dispersion.

⇒ Possibility for investigating Dirac's fermion physics!

Evidence of Dirac fermions?

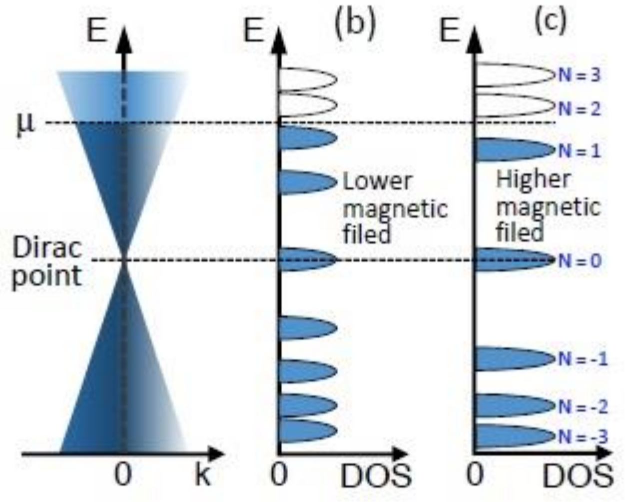
# QUANTUM OSCILLATIONS

- Electrons in strong B-field ⟶ Landau levels.




$$E = \left(N + \frac{1}{2}\hbar\omega\right) + \frac{\hbar^2 k_z^2}{2m} \longrightarrow \text{for } E(k) = \frac{\hbar^2 k^2}{2m}$$

For Dirac dispersion $E_{\pm}(k) = \pm v_f k$

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$$E_{\pm}(N) = \pm\sqrt{(2e\hbar v_f^2 B/c)N}$$

Periodic behavior of DOS.

⇓

Oscillations of physical quantities in 1/B!

$M$ ⟶ de Haas van Alphen oscillations.

$\sigma$ ⟶ Shubnikov de Haas oscillations.

# QUANTUM OSCILLATIONS

- de Haas van Alphen and Shubnikov de Haas oscillations (for 3D)

$$\Delta M = AR_T R_D R_s \sin\left[2\pi\left(\frac{F}{B}-\frac{1}{2}-\frac{1}{8}+\beta\right)\right]$$

$$\Delta\sigma_{xx} = AR_T R_D R_s \cos\left[2\pi\left(\frac{F}{B}-\frac{1}{2}-\frac{1}{8}+\beta\right)\right]$$

$2\pi\beta = \gamma$ Berry phase!

$$R_T = \frac{\frac{\alpha T}{B}}{\sinh\left(\frac{\alpha T}{B}\right)}$$

$$R_D = e^{-\frac{\alpha T_D}{B}}$$

$$R_S = \cos\left(\frac{\pi}{2} g \frac{m}{m_0}\right)$$

$$\alpha = 14.69 \frac{m}{m_0} TK^{-1}$$

Effective mass

$$F = \frac{\hbar}{2e} k_F^2$$

Informations about carrier density and Fermi surface snape.

$$T_D = \frac{\hbar}{2\pi k_B \tau}$$

Quantum scattering time

$$\gamma = i\oint_C d\vec{k}\left\langle\psi(\vec{k})\middle|\nabla_k\middle|\psi(\vec{k})\right\rangle$$

For Dirac fermions

$\gamma = \pi$

# SYNTHESIS

- Aim: high quality monocrystal samples.
  - The fewer impurities and defects ⟶ minimize the influence of bulk states and increase mobility.

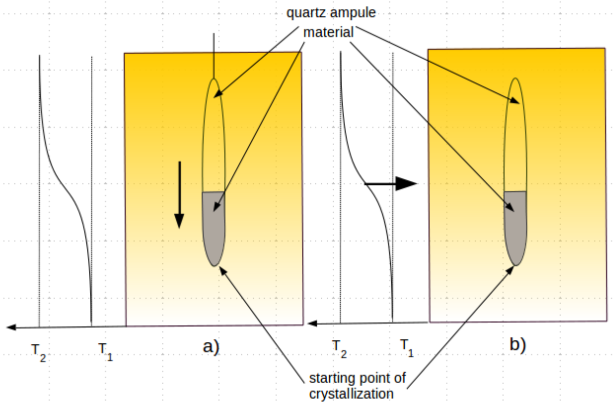
Sealing the quartz tube.

High vacuum in ampoule
- clean atmosphere
- volatile elements

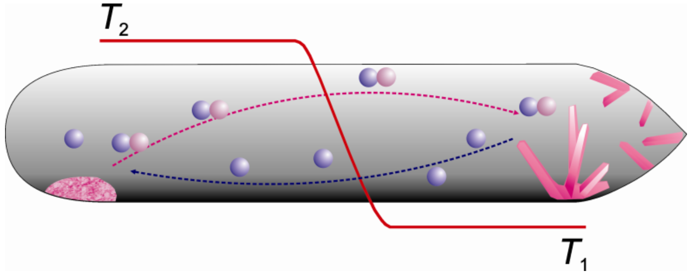
Material in vacuum seald quartz ampoule (vacuum $\sim 10^{-6}\ mbar$)

# SYNTHESIS

- Modified Bridgman method.




- (Chemical) vapor deposition.





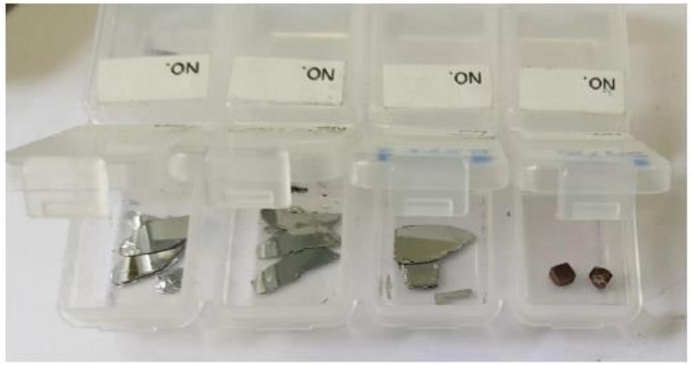
Temperature gradient is achieved by two-zone tube furnaces.

Synthesis parameters:
temperature, gradient, heating/cooling rate, growth time, amount and shape of material, ampoule dimensions.

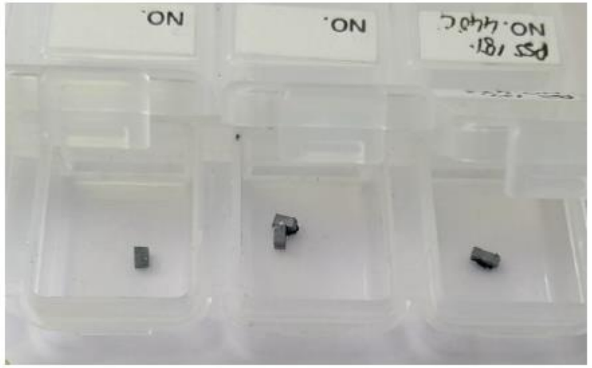
Optimization of parameters!

# SYNTHESIS

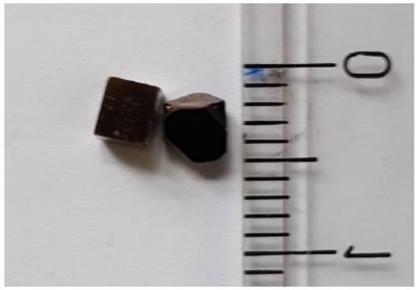
- Results of synthesis:



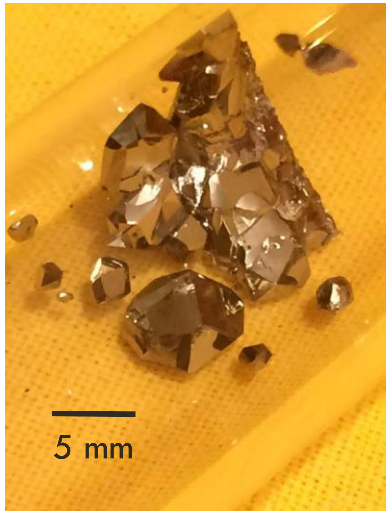
$BiSbTeSe_2$



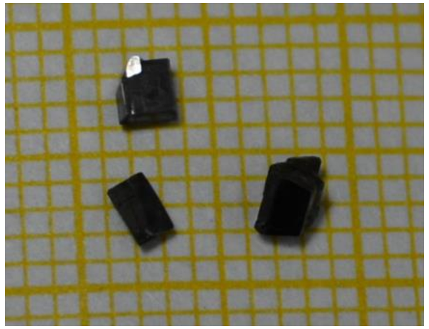
PbSnSe



SnTe



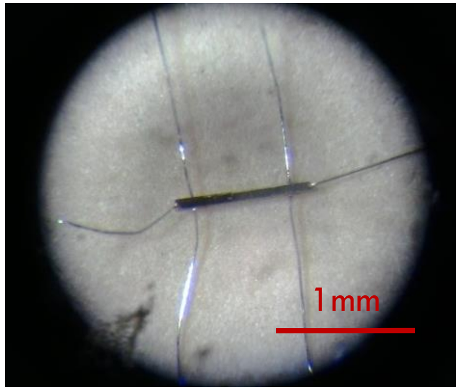

$Cd_3As_2$



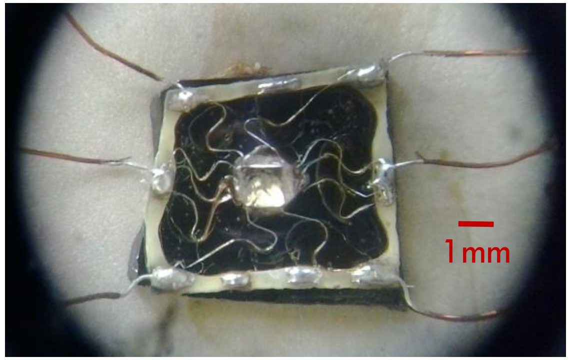
TaP

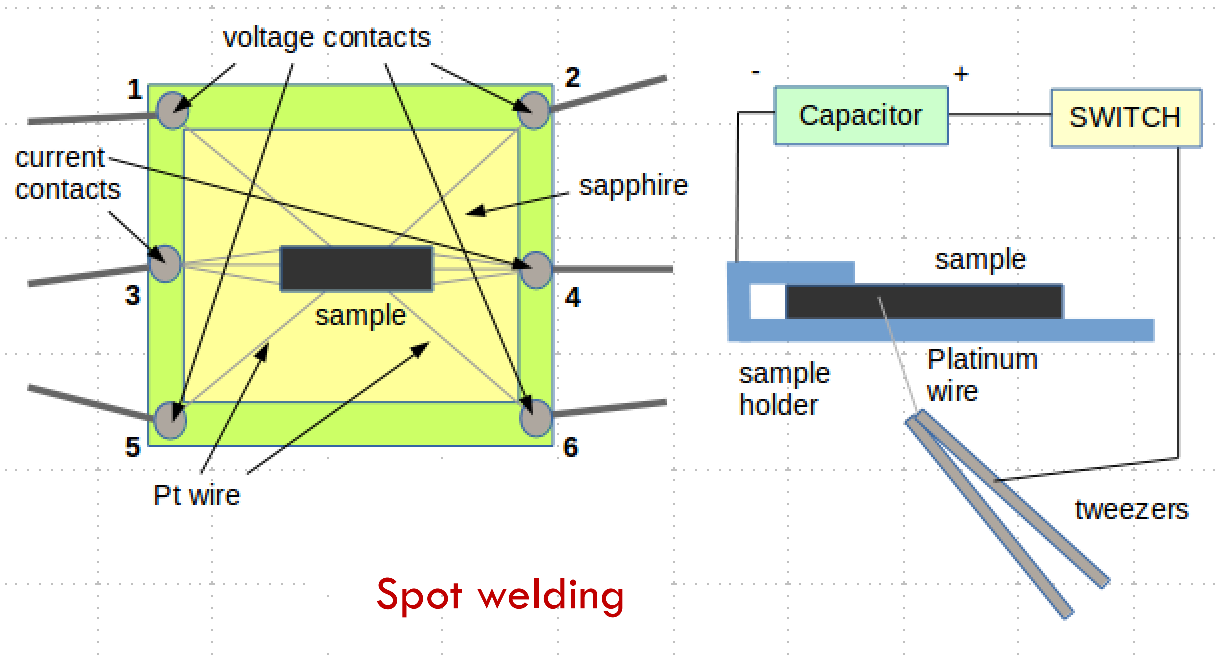
# SAMPLE PREPARATION

- For transport measurements good contacts are crucial (~ Ω).




Samples of $Cd_3As_2$ with contacts.



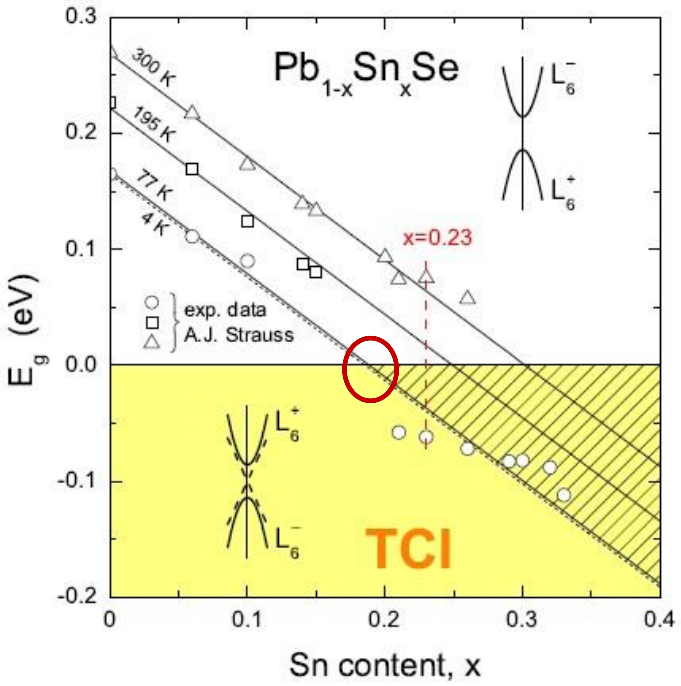

Spot welding

# PbSnSe

- $Pb_{1-x}Sn_xSe$ is a topological crystalline insulator for x > 0.23.
- Known for ages ⟶ energy gap depends on the T and x.

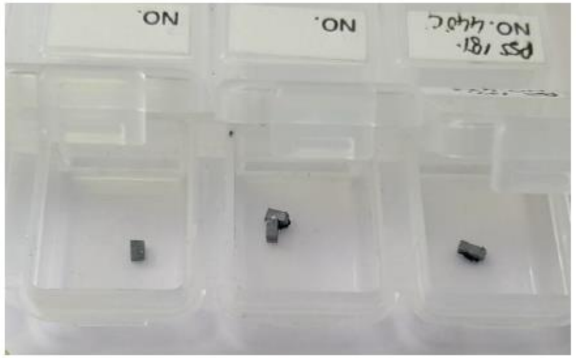
  ⟹ Topological phase transition with T or x.

- What happens at the transition point? ($x \approx 0.18$)



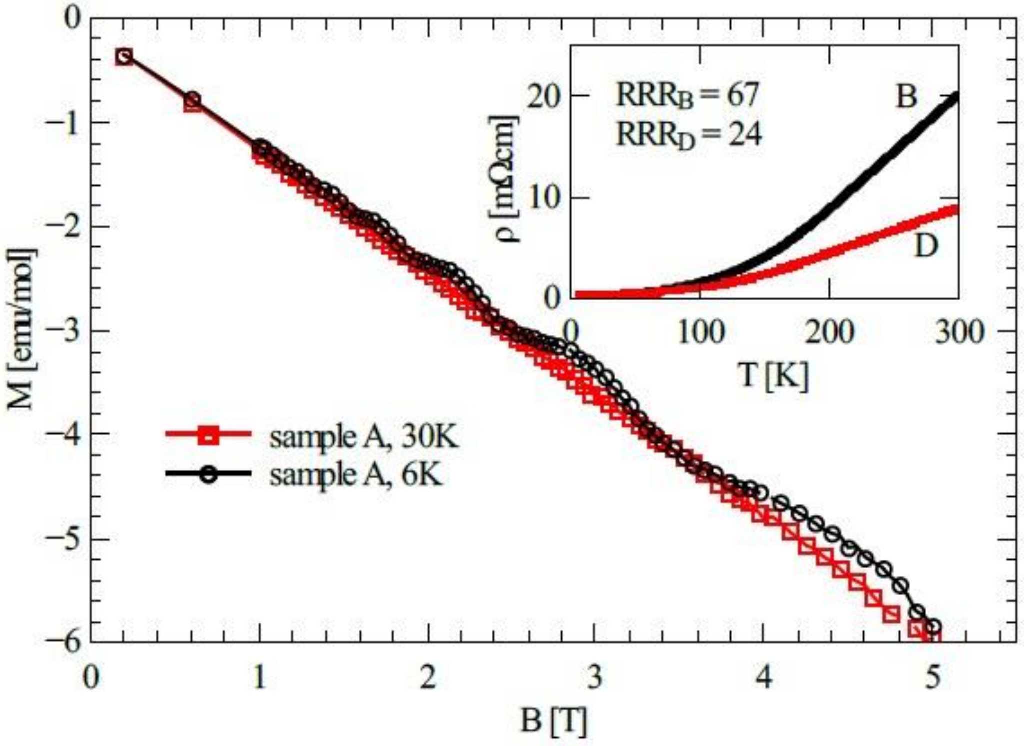


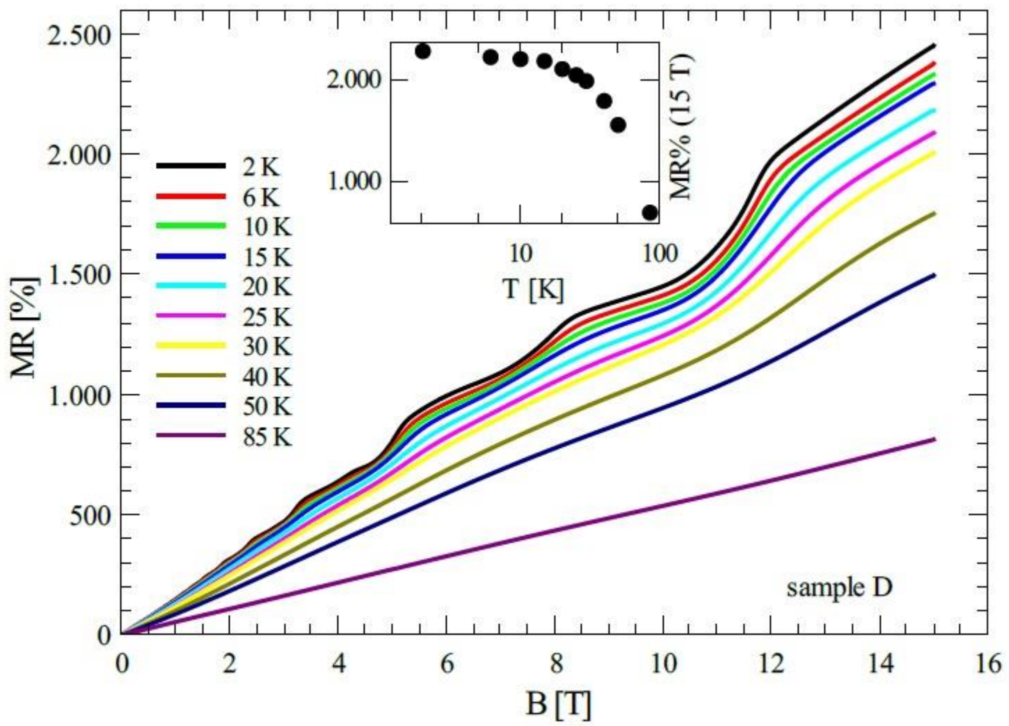

$x = 0.17, 0.18$



# PbSnSe

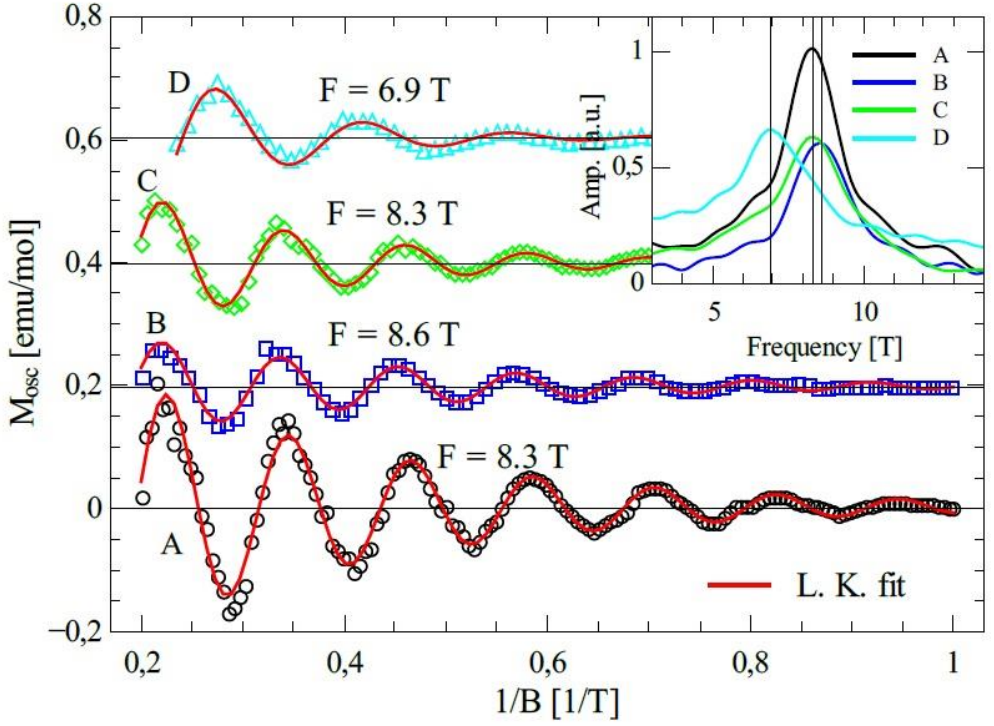
- Magnetization (SQUID) and magnetoresistance measurements in $Pb_{0.82}Sn_{0.18}Se$.



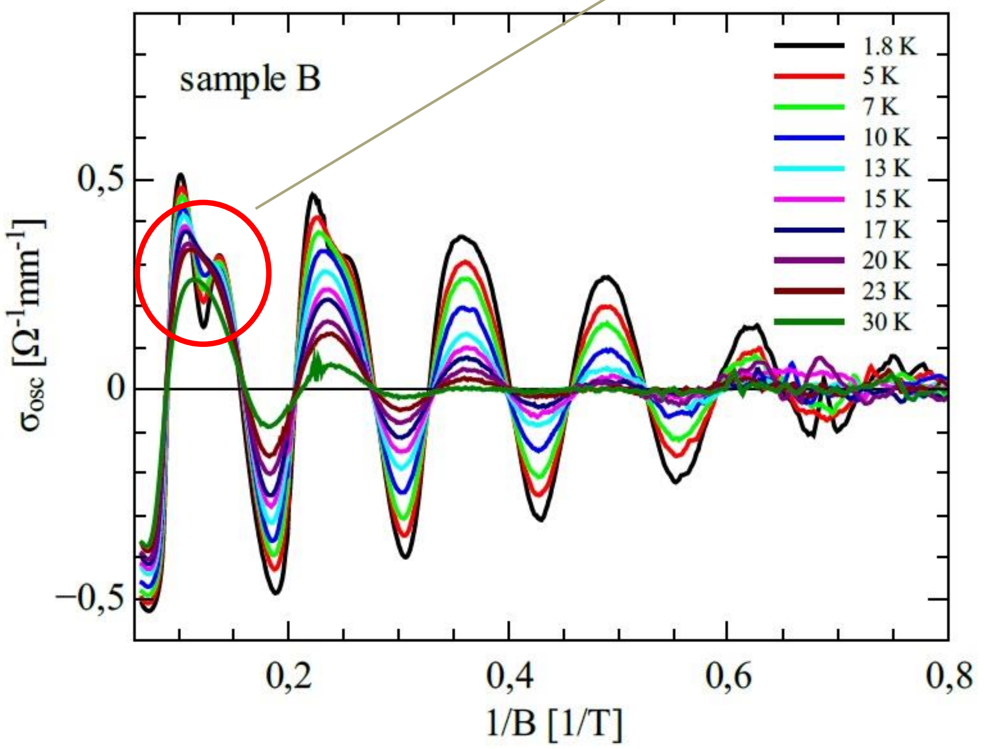



# PbSnSe

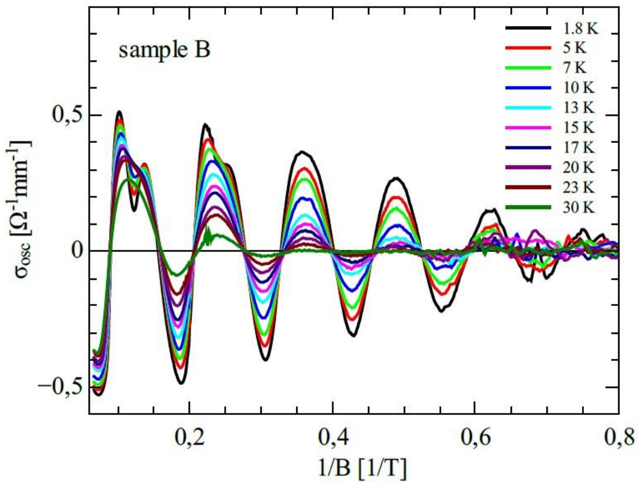
- By subtracting the background we get a pure oscillatory part.




Zeeman splitting of Landau levels.



# PbSnSe



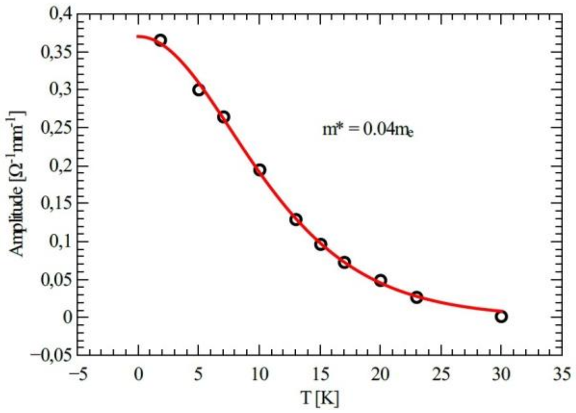

- How to get physical values from quantum oscillations?

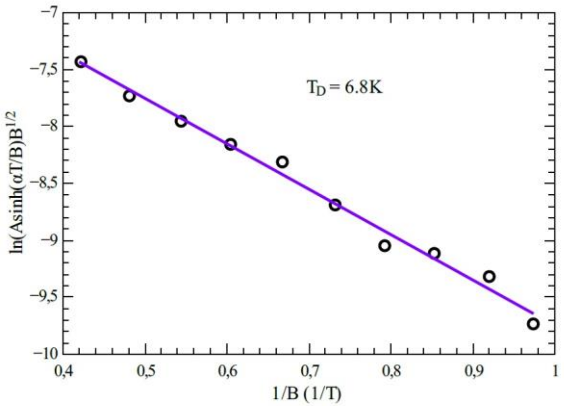
$$\Delta M = AR_T R_D R_s \sin\left[2\pi\left(\frac{F}{B}-\frac{1}{2}-\frac{1}{8}+\beta\right)\right]$$

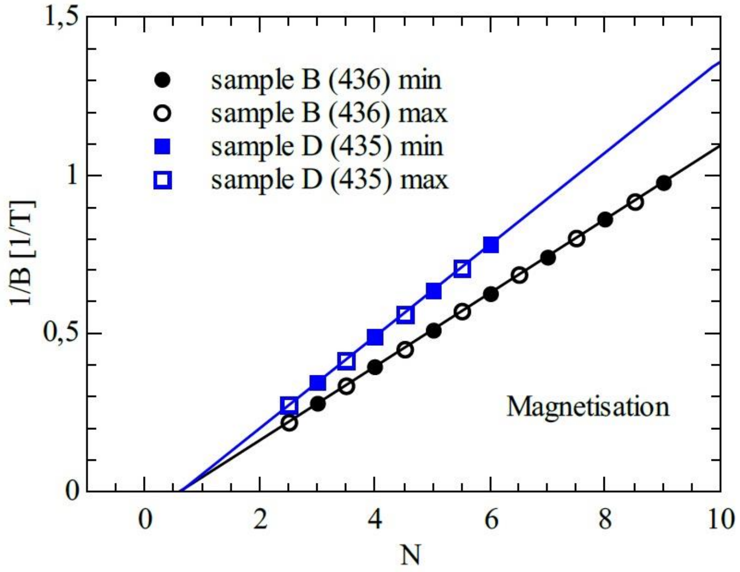
$$\Delta \sigma_{xx} = AR_T R_D R_s \cos\left[2\pi\left(\frac{F}{B}-\frac{1}{2}-\frac{1}{8}+\beta\right)\right]$$

$$R_T = \frac{\frac{\alpha T}{B}}{\sinh\left(\frac{\alpha T}{B}\right)}$$

$$R_D = e^{-\frac{\alpha T_D}{B}}$$

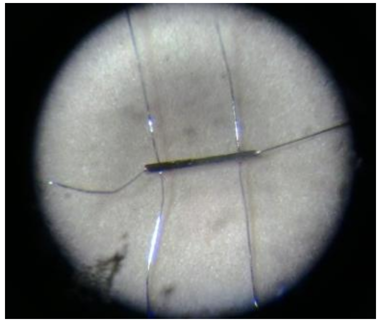


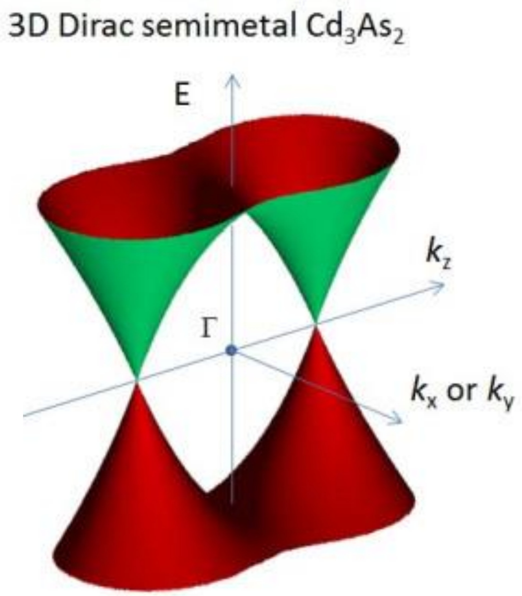




$$2\pi\left(\frac{F}{B}-\frac{1}{2}-\frac{1}{8}+\beta\right) = \pi\left(2N-\frac{1}{2}\right)$$

# $Cd_3As_2$



- $Cd_3As_2$ is an intrinsic (nontrivial) Dirac semimetal.
- Very stable material, except toxicity ideal for application and experiment.
- High mobility $\sim 10^6 cm^2 V^{-1} s^{-1}$.
- A pair of Dirac points in the direction of rotational symmetry axis ($k_z$).
- Anisotropy of Fermi surface? → Different frequencies for different direction of magnetic field.

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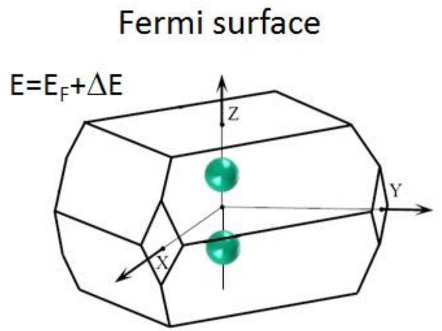


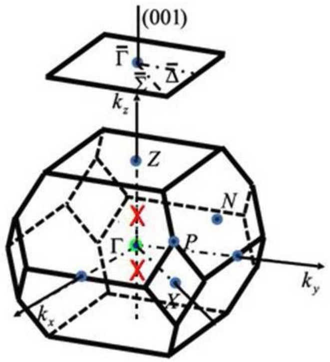


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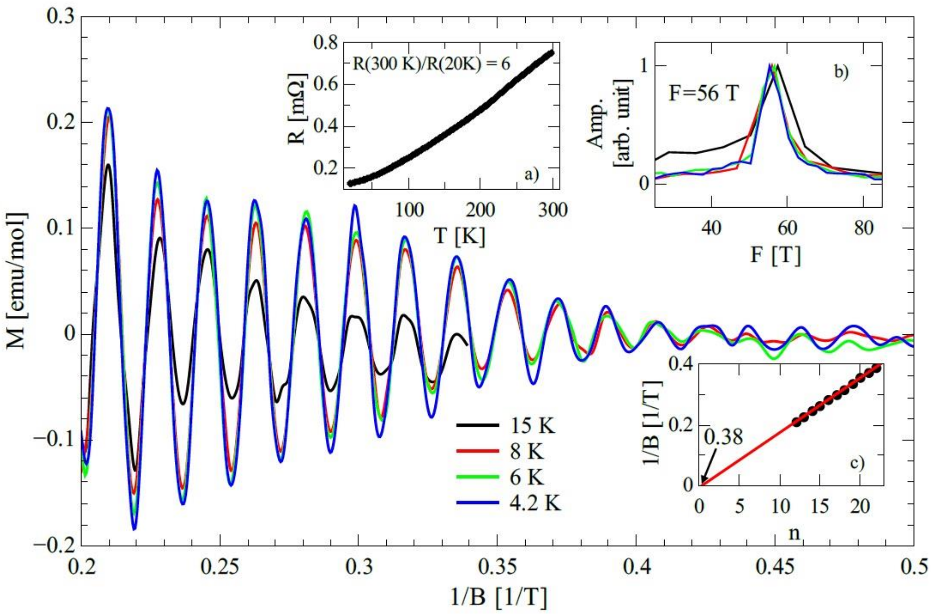
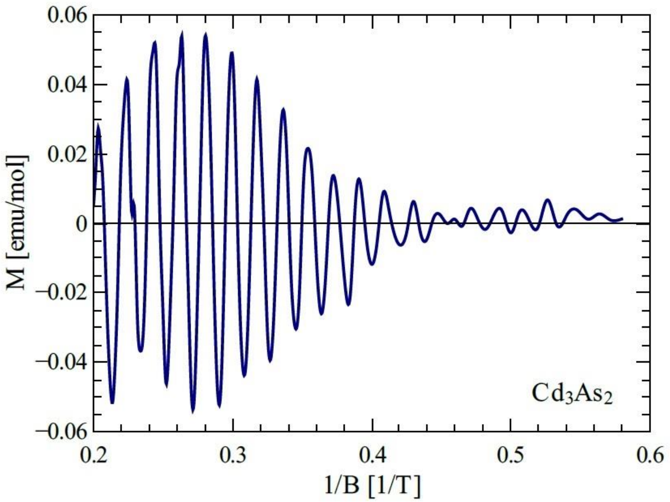
# $Cd_3As_2$

- Magnetization and magnetoresistance are measured.

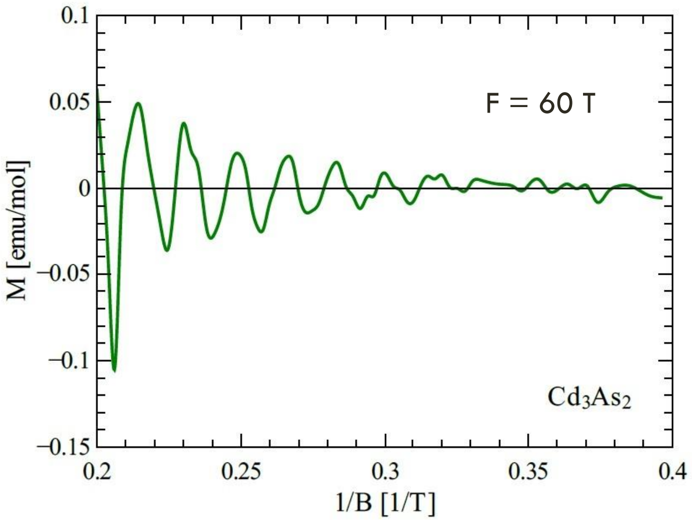



**B** in ab plane.




→ Superposition of frequencies.

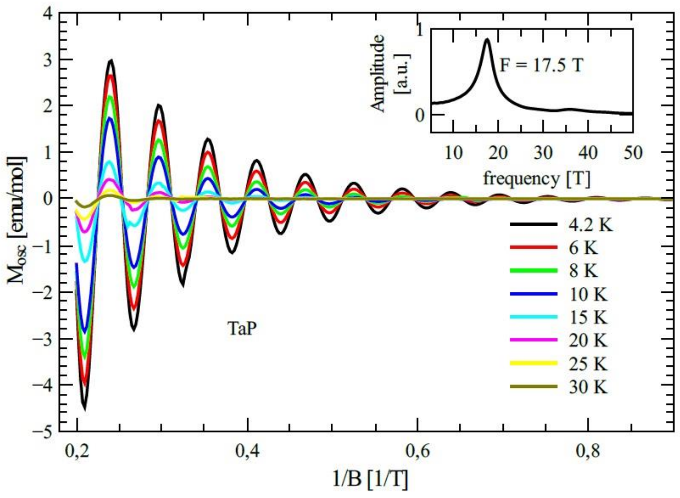
**B** perpendicular to ab plane.



# OTHER MATERIALS

- Other materials we have succsesfully synthesized:

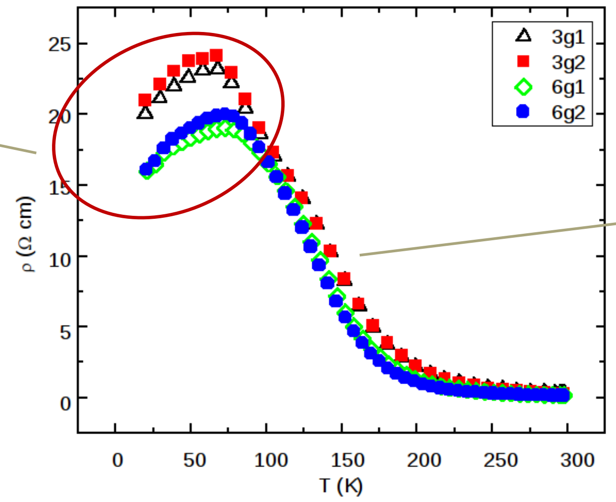
**TaP** → Weyl semimetal candidate.




Succsesfully observed quantum oscillations.

**$BiSbTe_2S$** → topological insulator.

Metallic behavior because off surface states.




Typical semiconducting behavior

# CONCLUSION

- Topological insulators.
  - symmetry protected surface states ⟶ spin locking and robustness at nonmagnetic impurities.

➡ An insight into the physics of Dirac 's fermions.

- Dirac semimetals.
  - 3D analogue of graphene. Symmetry protected Dirac points.

- The idea is to synthesize (determination of synthesis parameters) and characterize the obtained materials.

- Examine the consequences of the Dirac nature of cariers in magnetization and transport.